NBS MONOGRAPH 25—SECTION 21

U.S. DEPARTMENT OF COMMERCE/National Bureau of Standards

Standard X-ray Diffraction Powder Patterns

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- Metallurgy
- Reactor Radiation

[1] Headquarters and Laboratories at Gaithersburg, MD, unless otherwise noted; mailing address Gaithersburg, MD 20899.
[2] Some divisions within the center are located at Boulder, CO 80303
[3] Located at Boulder, CO, with some elements at Gaithersburg, MD.

Standard X-ray Diffraction Powder Patterns Section 21 — Data for 92 Substances

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Publications Available.

Previous work has been published as a book entitled Powder Diffraction Data from the Joint Committee on Powder Diffraction Standards Associateship at the National Bureau of Standards (1976) (obtainable from the publisher: JCPDS--International Center for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19081, price furnished on request). The volume is sold with an accompanying search manual, and contains 949 card images of patterns of experimental data, published originally as Circular 539 (vols. 1-10) and Monograph 25, Sections 1-12, and most of Section 13.

Individual copies of the Circular and Monograph are still available and may be obtained from the National Technical Information Service, 5285 Port Royal Road, Springfield, VA 22161. If a publication listed below is identified with a number, use this number in ordering. All are available in photocopy or microfiche; the price is not fixed and will be furnished on request.

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Volume 3	PB 178 904
Volume 4	PB 178 905
Volume 5	PB 178 906
Volume 6	PB 178 907
Volume 7	PB 178 908
Volume 8	PB 178 909
Volume 9	PB 178 910
Volume 10	PB 178 911

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ERRATA

Monograph 25

Section 17, p. 23: At d=1.4115M, change hkl=$\bar{2}2\bar{4}$ to $\bar{1}71$.
p. 23: At d=2.816, hkl should be $\bar{1}31$.

Section 19, p. 99: At entry "Niobium," delete the word "(monoclinic)."

Section 20, p. 58: Change formulas $Fe^{2}Nb_2O_6$ to $Fe^{+2}Nb_2O_6$.

Section 20, p. 130: At entry "Niobium," delete the word "(monoclinic)."

STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 21 Data for 92 Substances

by

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Standard x-ray powder diffraction patterns are presented for 92 substances. These patterns, useful for identification, were obtained by automated diffractometer methods. The lattice constants from the experimental work were refined by least-squares methods, and reflections were assigned hkℓ indices consistent with space group extinctions. Relative intensities, calculated densities, literature references, and other relevant data are included.

Key words: Crystal structure; densities; lattice constants; powder patterns; Pearson symbol; standard; x-ray powder diffraction.

INTRODUCTION

The Powder Diffraction File (PDF) is a continuing compilation of diffraction patterns gathered from many sources, produced, and published by the JCPDS--International Centre for Diffraction Data (JCPDS-ICDD)[1]. The PDF is used for identification of crystalline materials by matching d-spacings and diffraction intensity measurements. Under the partial sponsorship of the JCPDS, the program at the National Bureau of Standards contributes new or improved data to the PDF, and also aids in the development of diffraction techniques. This report presents information for 92 experimental patterns, and is the thirty-first of the series Standard X-ray Diffraction Powder Patterns[2].

EXPERIMENTAL POWDER PATTERNS

The nomenclature follows the current practice of the PDF. Common names are given when appropriate. In accord with the assignments of the JCPDS-ICDD mineral subcomittee, the mineral name, mineral group, and subgroup are given.

CAS registry number. The Chemical Abstracts Service Registry Number is included, when available, to help identify the sample. This number forms the basis for computer aided searching of Chemical Abstracts [Chemical Abstracts Service Registry Handbook--Number Section, 1974].

Sample. The samples used to make NBS patterns were obtained from a variety of sources or were prepared in small quantities in our laboratory. Appropriate annealing or recrystallization of the samples improved the quality of many of the patterns. A check of phase purity was provided by indexing the x-ray pattern.

Color. The names of the sample colors are selected from the ISCC-NBS Centroid Color Charts [1965].

Interplanar spacings. All spacing determinations were made using one or more internal standards mixed with the sample, packed in a shallow holder. Choice of the standard was determined by the need for low angle and unobstructed reflections. The amount of standard was estimated so that the intensity of its strongest peak would be about equal to the intensity of the strongest peak of the sample. The internal standards used were of high purity (99.99%). The calculated 2θ values used for them at 25°C are given in Tables 1 and 2; the 2θ angles were computed using cell dimensions uncorrected for index of refraction.

Standard Reference Material 640a [1982], Si powder (a=5.430825Å), was used for many patterns. The SRM 640a lattice constant for Si was refined from multiple powder data measurements made with tungsten and silver as internal standards. Single crystal cell parameter data were also collected. The lattice parameters from the two methods agreed within three parts in 10^5 [Hubbard, 1982]. D-values obtained using SRM 640a are in agreement with patterns recorded in this series of Monographs since 1966.

Another internal standard, fluorophlogopite (FP), is available as Standard Reference Material 675 [1982]. The d(001) spacing was refined from multiple powder data measurements using SRM 640a (Si) and tungsten as internal standards [Hubbard, 1983]. The calculated 2θ values of the 00ℓ lines are given in Table 2. Typically, only the low 2θ values (001-003) are used for calibration purposes.

[1] JCPDS--International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19081. This Pennsylvania non-profit corporation functions in co-operation with the American Ceramic Society, the American Crystallographic Association, the American Society for Testing and Materials, the Clay Minerals Society, the Institute of Physics, the Mineralogical Association of Canada, the Mineralogical Society of America, the Mineralogical Society of Great Britain and Ireland, the National Association of Corrosion Engineers, and the Société Française de Minéralogie et de Cristallographie.

[2] See previous page for other published volumes.

Table 1. Calculated 2θ angles for internal standards. CuKα, λ = 1.5405981A

hkℓ	Tungsten a=3.16524A ±.00004	Silver a=4.08651A ±.00002	Silicon a=5.430825A ±.000011 (SRM 640a)
110	40.262		
111		38.112	28.443
200	58.251	44.295	
211	73.184		
220	86.996	64.437	47.304
310	100.632		
311		77.390	56.124
222	114.923	81.533	
321	131.171		
400	153.535	97.875	69.132
331		110.499	76.378
420		114.914	
422		134.871	88.033
511/333		156.737	94.955
440			106.712
531			114.096
620			127.550
533			136.900
444			158.644

Table 2. Calculated 2θ angles for 00ℓ's. Internal standard fluorophlogopite, SRM 675.

$CuK\alpha_1$, λ = 1.5405981A, d_{001} = 9.98104A (±0.00007)	
00ℓ	2θ
1	8.853
2	17.759
3	26.774
4	35.962
5	45.397
6	55.169
7	65.399
8	76.255
10	101.025
11	116.193
12	135.674

All data were collected at room temperature on a diffractometer equipped with a focusing graphite crystal monochromator located betwen the sample and the scintillation counter. Pulse height discrimination was used as well. The data were collected using copper radiation: λ($CuK\alpha_1$, peak) = 1.5405981A [Deslattes and Henins, 1973].

All of the patterns reported in this monograph were measured with a computer controlled diffractometer. Digital data were measured on one of two diffractometers controlled by the AUTO program [Snyder et al., 1981]. The patterns were measured in step-scan mode with a step width of 0.01 degrees and counting times at each point greater than or equal to 3 seconds except when reactivity required more rapid data collection.

The data were processed with the JCPDS-NBS POWDER-PATTERN system of programs [Pyrros and Hubbard, 1983]. First the raw data were processed by the program POWDER.PATTERN that locates peaks with the second derivative algorithm of Savitzky and Golay [1964]. A three point Newton-Gregory interpolation [Daniels, 1978] was used to locate the derivative minimum. Peaks hidden by lines of the internal standard were read from strip chart recordings. For some patterns, weak peaks were located with the interactive graphics program PLOT.PATTERN/INT. This program displays the spectrum on a Tektronix graphic terminal. The user can locate peaks by positioning a cursor at the peak. The peak position is defined either as the position of the cursor or as the minimum of the second derivative nearest to the cursor. The $K\alpha_2$ peaks were occasionally read to assist in establishing a $K\alpha_1$ peak position, but $K\alpha_2$ peaks are not reported.

All patterns were plotted on paper with the program PLOT.PATTERN/HRD on a scale of one degree per inch and were visually inspected. The program POWDER.CALIBR was used to calculate a polynomial correction curve. This was done in two stages: first an external calibration (instrument 2θ correction) was obtained to correct the observed internal standard positions; second, from those positions and their theoretical positions the polynomial curve was derived and applied to all peaks of the pattern. At low angles, $K\alpha_1$ and $K\alpha_2$ peaks were unresolved for both the sample and the internal standard. Internal standard corrections were established from the theoretical values for $K\alpha_1$ and were applied to the unresolved low angle peaks, as well as to the resolved $K\alpha_1$ peaks in the higher angle regions. The program POWDER.EDTPKS was used to flag reflections to be used in the least-squares cell parameter refinement. Reflections due to $CuK\alpha_2$ radiation were excluded from the refinement.

Structure, lattice constants. The space group symbols are given in the short Hermann-Mauguin notation. Also given are the space group numbers listed in the International Tables for X-ray Crystallography, Vol. I [1965]. When the space group symbol is not known, the lattice centering symbol or the diffraction aspect for the Laue class may be given [Donnay and Kennard, 1964; Mighell et al., 1981].

The given Pearson symbol is generated by computer [Hubbard and Calvert, 1981].

Orthorhombic cell dimensions are arranged according to the Dana convention b>a>c [Palache et al., 1944]. Monoclinic and triclinic lattice constants are transformed, if necessary, in order to follow the convention of Crystal Data [1973]. The lattice constant ratios, a/b, c/b, and c/a, also follow the conventions used for the determinative ratios in Crystal Data [1973].

In most cases, preliminary lattice constants were available in the literature, and were used for the initial indexing and refinement. In cases where such data were not available, other methods were tried. If suitable single crystals were available, the lattice constants were obtained by use of a four-circle diffractometer. Axial ratios and densities from Groth [1908] were sometimes useful. Cell constants were also found in some instances by use of Visser's computer program, Ito 9 [Visser, 1969].

A least squares program, JCPDS-NBS*LSQ82, derived from the program of Evans, Appleman, and Handwerker [1963], assigned hkℓ's and refined the lattice constants. The cell refinement was based only upon corrected 2θ values ($2\theta_{corr}$) which could be indexed without ambiguity. The program minimized the value $\sum(\theta_{corr}-\theta_{calc})^2$. Generally, when two or more calculated 2θ's were within 0.03 degrees of the corrected 2θ, the index giving the best fit was reported. An editorial flag ,+, indicates that 2 or more indices were possible. Multiple hkℓ's were not utilized or reported in indexing cubic patterns. Instead, a single appropriate index was used.

The estimated standard deviations (e.s.d.'s) of the reciprocal cell parameters were determined from the inverse matrix of the normal equations. The program calculated the e.s.d.'s of the direct cell constants by the method of propagation of errors. Since 1973, the e.s.d.'s derived by the computer program have been increased by 50% in order to reflect more truly the uncertainty in the lattice constants. A similar increase should also be applied to all lattice constants published in this series of NBS publications prior to 1973. The e.s.d.'s in the least significant figures are given in parentheses following the lattice constants.

For each d-value, the number of significant figures was derived from the average error in $|2\theta_{corr}-2\theta_{calc}|$ and the equation $\Delta d/d = -(\cot\theta)\overline{\Delta\theta}$. With these conditions, the rounded value of d agrees with its appropriate 2θ within the average error in 2θ. The value of $\overline{\Delta\theta}$ varies with the symmetry and crystallinity of each sample.

Densities. These were calculated from the specified lattice constants, the Avogadro number 6.0220943×10^{23} [Deslattes et al., 1974] and the 1977 atomic weights published by the International Union of Pure and Applied Chemistry [1979].

Figures of merit. Several figures of merit ratings are available for assessing indexed powder data. M_{20} [de Wolff, 1968] is a criterion for the reliability of the unit cell and indexing. M_{20} is defined by:

$$M_{20} = \frac{Q_{20}}{2\bar{\varepsilon}\ N_{20}}$$

where Q_{20} is the value of $1/d^2$ for the 20th observed line (not counting unexplained lines), N_{20} is the number of different calculated Q values up to Q_{20}, and $\bar{\varepsilon}$ is the average magnitude of the discrepancy in Q for these 20 lines. A value of $M_{20} > 10$ will guarantee the essential correctness of the indexing provided there are not more than 2 spurious lines ($X_{20} \leq 2$) [de Wolff, 1968]. The number of unindexable lines occurring up to the 20th observed and indexed line is X_{20}. In general, patterns reported in this publication had $M_{20} > 20$ and $X_{20} = 0$.

The accuracy and completeness of the measured interplanar spacings is conveniently reported using the format:

$$F_N = \text{overall value } (\overline{|\Delta 2\theta|}\ , N_{poss}).$$

The "overall" value is the figure of merit of Smith and Snyder [1979] defined by:

$$\frac{1}{\overline{|\Delta 2\theta|}} \cdot \frac{N}{N_{poss}} .$$

N, the number of observed reflections, was chosen as 30 or as the maximum number of lines of the pattern if the pattern had fewer than 30 lines. $\overline{\Delta 2\theta}$ is the average absolute magnitude of the discrepancy between observed and calculated 2θ values for each reported hkℓ. N_{poss} is the number of diffraction lines allowed in the space group, up to the N^{th} observed and indexed line. Co-positional lines such as the cubic 221 and 300 are counted as one possible line.

Intensity measurements. The intensities of the diffraction lines were measured as peak heights above background and were expressed relative to the strongest line. It has been found that samples which give satisfactory intensity patterns usually have an average particle size smaller than 10 μm, as recommended by Alexander et al. [1948]. In order to avoid the orientation effects which occur when powdered samples are packed or pressed, a sample holder was made that had in its top face a rectangular cavity which extended to one end of the holder. To prepare the sample, a glass slide was clamped over the top face to form a temporary cavity wall (see fig. 1), and the powdered sample was allowed to drift into the end opening while the holder was held in a vertical position.

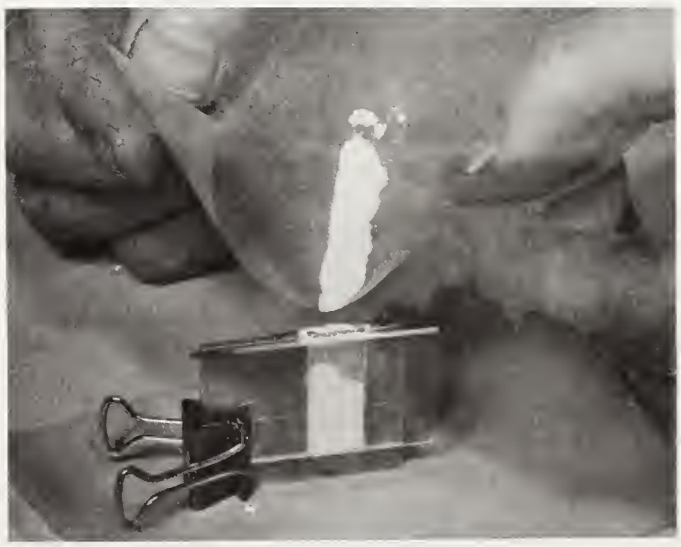

Figure 1. Loading an intensity sample.

With the sample holder returned to a horizontal position, the glass slide was carefully removed so that the sample could be exposed to the x-ray beam (see fig. 2).

Figure 2. Cover slide removed from intensity sample.

As a general practice, approximately 50 volume percent of finely ground silica gel was added as a diluent. Occasionally, a rotating sample holder was used.

As a check on reproducibility, each sample was loaded at least 3 times. The intensity values were determined for each of the mountings. The reported I^{rel} value for each observed spacing is the average of 3 or more observations and is rounded to the nearest integer. For patterns with high angle lines, the intensities of lines with 2θ above 70° were measured only once. Theta-compensating (variable divergence) slits were sometimes used to gather the intensity data. In that case, the average I(comp) for each spacing was converted to an equivalent fixed slit value, using the approximate equation:

$$I(\text{fixed}) = \frac{I(\text{comp})}{\sin\theta} .$$

The estimated standard deviation, σ, in the relative intensity values was calculated from the values of the five strongest lines, excluding the line with $I^{rel} = 100$.

$$\sigma_i^2 = \frac{1}{n-1} \sum_{k=1}^{n} (I_i^{rel}(k) - \langle I \rangle_i)^2$$

and

$$\sigma = \left(\frac{1}{m} \sum_{i=1}^{m} \sigma_i^2 \right)^{\frac{1}{2}}$$

where

i is one of the strong lines
m is the number of strong lines (usually 5), and
n is the number of independent observations, per line.

Where conversion of intensities for effects of theta-compensating slits was required, each σ_i was multiplied by the conversion factor

$$f = \frac{I(\text{comp})}{I(\text{fixed})} .$$

UNITS

In this publication the Angström unit (1Å=100pm) was selected for presentation of the d-value and lattice parameters. This maintained consistency with (a) the series of earlier publications of Standard X-ray Diffraction Powder Patterns (see pg. iv); (b) the publications of the International Union of Crystallography; and (c) the continuing publication of cards and search manuals of the PDF (now consisting of over 42,000 entries). The PDF search manuals are based on the d-values in Å of the 3 strongest lines. Consistent with the choice of the Å unit for length, the volume of the unit cell is expressed in $Å^3$($1\ Å^3 = 1 \times 10^{-30}\ m^3$). Densities are reported in g/cm^3 ($1\ gm/cm^3 = 10^3\ kg/m^3$).

COMPUTER ASSISTED PUBLICATION

In Sections 16 through 20 the d/I/hkℓ tables were prepared by computer transfer of the data. Beginning with Section 21, the entire report was generated from the NBS*AIDS83 database. This change resulted in a few changes in the layout as well as the addition of a few supplemental data items such as Pearson Symbol, the figure of merit (M_{20})for all patterns, and largest d-value examined in data collection. In addition, in order to transfer the database elements to the JCPDS without major revision the references are now indicated by number (e.g., #1) instead of by author and year.

ACKNOWLEDGMENTS

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Wolff, de, P. M. (1968). J. Appl. Crystallogr. 1, 108.

Aluminum Carbide, Al_4C_3

CAS registry no.
1299-86-1

Sample
The sample was obtained from Materials Research Corp., Orangeburg, NY.

Color
Dark greenish yellow brown

Symmetry classifications

Crystal System	Rhombohedral
Space Group	$R\bar{3}m$ (166)
Pearson Symbol	hR7

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	Ag FP
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±5

Crystallographic constants of this sample
(Hexagonal axes)
a = 3.3388 (3) A
c = 24.996 (3)

c/a = 7.4865

V = 241.31 A^3
Z = 3
Density (calc.) = 2.972 g/cm^3

Figures of merit
F_{29} = 61.4(.0121, 39)
M_{20} = 83.4

Comments
The structure was determined by Jeffrey and Wu (#1).
The mean temperature of data collection was 23.9°C.

Additional patterns
PDF card 11-629

Reference
#1. Jeffrey, G.A. and Wu, V.Y.
Acta Crystallogr.(1966) 20,538.

d(A)	I^{rel}	hkl	2θ(°)
8.34	2	0 0 3	10.604
4.167	10	0 0 6	21.305
2.872	54	1 0 1	31.113
2.817	100	0 1 2	31.740
2.775	13	0 0 9	32.233
2.503	54	0 1 5	35.850
2.248	83	1 0 7	40.085
2.122	10	0 1 8	42.575
2.082	49	0 0 12	43.431
1.8911	23	1 0 10	48.075
1.7874	13	0 1 11	51.057
1.6670	86	0 0 15	55.043
1.6007	1L	1 0 13	57.532
1.5494	1L	1 1 6	59.624
1.5195	18	0 1 14	60.921
1.4430	4	0 2 1	64.525
1.4361	10	2 0 2	64.875
1.4304	6	1 1 9	65.166
1.3890	9	2 0 5+	67.362
1.3746	1L	1 0 16	68.163
1.3402	11	0 2 7	70.164
1.3108	10	0 1 17	71.979
1.3031	28	1 1 12	72.477
1.2515	3	0 2 10	75.980
1.2195	2	2 0 11	78.342
1.1972	5	1 0 19	80.091
1.1236	5	2 0 14	86.555
1.0918	3	2 1 1	89.745
1.0889	7	1 2 2	90.047

Aluminum Fluoride Hydrate, β-$AlF_3 \cdot 3H_2O$

Synonym
Aluminum trifluoride trihydrate

CAS registry no.
15098-87-0

Sample
The sample was obtained from the Aesar Division of Johnson Matthey, Inc., Seabrook, NH.

Color
Colorless

Symmetry classifications
Crystal System Tetragonal
Space Group P4/ncc (130)
Pearson Symbol tP52

Data collection and analysis parameters
Radiation $CuK\alpha_1$
Wavelength 1.5405981 A
2θ Standards W FP
Scanned to 5.0° 2θ
$\sigma(I^{rel})$ ±2

Crystallographic constants of this sample
a = 7.7207 (4) A
c = 7.2979 (7)

c/a = 0.9452

V = 435.02 A^3
Z = 4
Density (calc.) = 2.107 g/cm^3

Figures of merit
F_{30} = 90.1 (.0067, 50)
M_{20} = 100.8

Comments
The unit cell and space group were determined by Freeman (#1).
A hexagonal alpha-form has also been described by Ehret and Frere (#2).
The temperature of data collection was approximately 25.0°C.

Additional patterns
PDF card 9-108

References
#1. Freeman, R.D.
J. Phys. Chem.(1956) 60,1152.
#2. Ehret, W.F. and Frere, F.J.
J. Am. Chem. Soc.(1945) 67,64.

d(A)	I^{rel}	hkl	2θ(°)
5.460	100	1 1 0	16.221
3.860	47	2 0 0	23.021
3.648	16	0 0 2	24.378
3.299	41	1 0 2	27.006
3.033	27	1 1 2	29.421
2.729	21	2 2 0	32.793
2.651	16	2 0 2	33.781
2.5075	19	2 1 2	35.781
2.4412	39	3 1 0	36.787
2.1855	7	2 2 2	41.275
2.1034	2	3 0 2	42.964
2.0292	16	3 1 2	44.619
1.9296	11	4 0 0	47.057
1.8466	8	3 2 2	49.308
1.8194	4	3 3 0	50.097
1.7752	25	1 0 4	51.434
1.7263	32	4 2 0	53.001
1.6656	6	4 1 2	55.094
1.6283	3	3 3 2	56.469
1.6131	7	2 1 4	57.048
1.5600	3	4 2 2	59.179
1.5141	6	5 1 0	61.162
1.4883	2	3 0 4	62.337
1.4615	2	3 1 4	63.613
1.4220	2	4 3 2	65.601
1.3984	4	5 1 2	66.848
1.3889	10	3 2 4	67.366
1.3646	1L	4 4 0	68.732
1.3346	4	5 2 2	70.507
1.3242	3	5 3 0	71.143
1.3070	8	4 1 4	72.224
1.2786	1	4 4 2	74.092
1.2446	3	5 3 2	76.476
1.2209	6	6 2 0	78.236
1.2136	2	6 0 2	78.799
1.2016	1	1 0 6	79.745
1.1989	2	6 1 2	79.961
1.1785	6	4 3 4	81.628
1.1651	1L	5 1 4	82.773
1.1576	1L	6 2 2	83.428
1.1452	1L	5 4 2	84.545
1.1274	5	5 2 4	86.197

Ammonium Fluoride, NH_4F

CAS registry no.
12125-01-8

Sample
The sample was obtained from British Drug Houses, Ltd., Poole, England. There was a small amount of ammonium hydrogen fluoride present.

Color
Colorless

Symmetry classifications
Crystal System Hexagonal
Space Group $P6_3mc$ (186)
Pearson Symbol hP12

Data collection and analysis parameters
Radiation $CuK\alpha_1$
Wavelength 1.5405981 A
2θ Standard Ag
Scanned to 17.7° 2θ
$\sigma(I^{rel})$ ±6

Crystallographic constants of this sample
a = 4.4408 (2) A
c = 7.1726 (6)

c/a = 1.6152

V = 122.50 A^3
Z = 2
Density (calc.) = 1.004 g/cm^3

Figures of merit
F_{30} = 69.7(.0110, 39)
M_{20} = 126.6

Comments
The structure was determined by Zachariasen (#1). There is a cubic form at 4 kbar and 177°C (#2) and various other unindexed high pressure - low temperature forms (#3).
The mean temperature of data collection was 24.2°C.

Additional patterns
PDF card 8-32

References

#1. Zachariasen, W.H.
Z. Phys.(1927) 127,218.
#2. Calvert, L.D. and Whalley, E.
J. Chem. Phys.(1970) 53,2151.
#3. Nabar, M.A. et al.
J. Chem. Phys.(1969) 51,1353.

d(A)	I^{rel}	hkl	2θ(°)
3.847	100	1 0 0	23.103
3.588	44	0 0 2	24.796
3.391	53	1 0 1	26.262
2.623	22	1 0 2	34.155
2.222	42	1 1 0	40.572
2.0298	30	1 0 3	44.605
1.9234	4	2 0 0	47.218
1.8874	17	1 1 2	48.173
1.8570	5	2 0 1	49.015
1.7937	1L	0 0 4	50.865
1.6954	2	2 0 2	54.046
1.6251	1L	1 0 4	56.587
1.4986	7	2 0 3	61.862
1.4538	3	2 1 0	63.991
1.4244	3	2 1 1	65.474
1.3947	1L	1 1 4	67.050
1.3441	3	1 0 5	69.935
1.2821	3	3 0 0	73.858
1.2419	3	2 1 3	76.668
1.2071	1	3 0 2	79.303
1.1952	1L	0 0 6	80.253
1.1499	1	2 0 5	84.117
1.1104	1L	2 2 0	87.851
1.0666	1L	3 1 0	92.477
1.0606	1L	2 2 2	93.148
1.0549	1L	3 1 1	93.809
1.0528	1L	1 1 6	94.049
1.0210	1L	2 1 5	97.954
1.0152	1L	2 0 6	98.704
0.9741	1	3 1 3	104.512
0.9617	1L	4 0 0	106.454
0.9528	1L	4 0 1	107.886
0.9232	1L	2 1 6	113.102
0.9043	1L	2 0 7	116.815
0.89196	1L	4 0 3	119.448

Ammonium Iron Sulfate Hydrate, $(NH_4)_2Fe(SO_4)_2 \cdot 6H_2O$

Mineral name
Mohrite, syn
Picromerite Group

CAS registry no.
7783-85-9

Sample
The sample was made by slow evaporation of an aqueous solution of $FeSO_4$ and $(NH_4)_2SO_4$.

Color
Very light bluish green

Symmetry classifications

Crystal System	Monoclinic
Space Group	$P2_1/a$ (14)
Pearson Symbol	mP78
Structure Type	A Tutton salt

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	FP Ag
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±3

Crystallographic constants of this sample

a = 9.2924 (17) A
b = 12.601 (3)
c = 6.2491 (13)
β = 106.792 (16)°

a/b = 0.7374
c/b = 0.4959

V = 700.53 A^3
Z = 2
Density (calc.) = 1.859 g/cm^3

Figures of merit
F_{30} = 74.6(.0106, 38)
M_{20} = 42.5

Comments
The structure of a Tutton salt, $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$, was determined by Margulis and Templeton (#1).
The mean temperature of data collection was 23.8°C.

Additional patterns
PDF card 17-481

References
#1. Margulis, T.N. and Templeton, D.H. Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.(1962) 117,334.

d(A)	I^{rel}	hkl	2θ(°)
7.28	2	1 1 0	12.154
6.310	9	0 2 0	14.023
5.990	9	0 0 1	14.776
5.408	35	0 1 1	16.379
5.277	6	-1 1 1	16.788
5.148	15	1 2 0	17.211
4.452	16	2 0 0	19.927
4.337	20	0 2 1	20.461
4.265	35	-1 2 1	20.813
4.196	100	-2 0 1+	21.155
4.163	42	1 1 1	21.328
3.982	6	-2 1 1	22.308
3.801	75	1 3 0	23.384
3.635	9	2 2 0	24.469
3.612	9	1 2 1	24.625
3.491	4	-2 2 1	25.494
3.438	13	0 3 1	25.894
3.403	17	-1 3 1	26.162
3.161	18	2 0 1	28.209
3.150	21	0 4 0	28.306
3.066	22	2 1 1	29.101
3.029	47	-1 1 2	29.470
2.969	3	-2 3 1+	30.079
2.945	2	-3 1 1	30.323
2.902	10	-2 0 2	30.790
2.887	10	3 1 0	30.952
2.826	25	-2 1 2	31.638
2.797	24	-1 2 2	31.972
2.769	4	-1 4 1	32.300
2.729	10	-3 2 1	32.789
2.686	1L	3 2 0	33.331
2.635	2	-2 2 2	33.992
2.571	9	2 4 0	34.868
2.562	9	1 1 2+	34.993
2.526	8	2 3 1	35.513
2.456	32	-3 3 1	36.557
2.436	5	0 3 2	36.875
2.424	2	1 5 0+	37.054
2.386	8	-2 3 2	37.674
2.322	2	0 5 1+	38.743
2.230	1	2 4 1	40.414
2.190	6	4 1 0	41.189
2.185	7	-3 4 1	41.284
2.169	16	0 4 2	41.597
2.158	8	3 4 0	41.816
2.133	6	-2 4 2	42.336
2.0974	14	4 2 0+	43.093
2.0523	3	-1 1 3	44.090
2.0282	8	-2 1 3	44.641
1.9910	7	-4 2 2	45.523
1.9824	4	0 6 1	45.730
1.9697	3	0 1 3+	46.042
1.9375	3	-3 5 1	46.852
1.9204	7	3 5 0	47.296
1.9125	10	4 0 1	47.504

continued

Ammonium Iron Sulfate Hydrate, $(NH_4)_2Fe(SO_4)_2 \cdot 6H_2O$ (continued)

d(A)	I^{rel}	hkl			2θ(°)
1.8982	4	2	6	0	47.882
1.8776	3	-4	3	2+	48.442
1.8648	4	-4	4	1	48.797
1.8457	3	-2	3	3	49.334
1.8378	4	-5	1	1	49.560
1.8294	2	4	2	1	49.805
1.8166	6	1	1	3+	50.180
1.8057	5	2	4	2	50.502
1.8013	3	0	3	3	50.636
1.7742	3	-3	5	2	51.464
1.7622	3	1	2	3+	51.840
1.7404	6	4	3	1	52.540
1.7362	6	3	5	1	52.675

Ammonium Magnesium Selenate Hydrate, $(NH_4)_2Mg(SeO_4)_2 \cdot 6H_2O$

Sample
The sample was prepared by slow evaporation of an aqueous 1:1 molar solution of $(NH_4)_2SeO_4$ and $MgSeO_4$ at room temperature.

Color
Colorless

Symmetry classifications

Crystal System	Monoclinic
Space Group	$P2_1/a$ (14)
Pearson Symbol	mP78
Structure Type	A Tutton salt

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	FP Ag
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±4

Crystallographic constants of this sample

a = 9.471 (1) A
b = 12.7657 (18)
c = 6.3374 (7)
β = 106.476 (11)°

a/b = 0.7419
c/b = 0.4964

V = 734.75 A^3
Z = 2
Density (calc.) = 2.054 g/cm^3

Figures of merit

F_{30} = 98.2(.0069, 44)
M_{20} = 57.0

Comments
The structure of a Tutton salt, $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$, was determined by Margulis and Templeton (#1). The mean temperature of data collection was 23.9°C.

Additional patterns
PDF card 28-74

Reference
#1. Margulis, T.N. and Templeton, D.H. Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.(1962) 117,334.

d(A)	I^{rel}	hkl	2θ(°)
7.410	18	1 1 0	11.934
6.383	2	0 2 0	13.862
6.081	2	0 0 1	14.555
5.494	60	0 1 1	16.121
5.346	16	-1 1 1	16.569
5.225	28	1 2 0	16.957
4.543	15	2 0 0	19.525
4.401	17	0 2 1	20.159
4.326	74	-1 2 1	20.512
4.266	100	-2 0 1	20.804
4.044	10	-2 1 1	21.961
3.854	64	1 3 0	23.059
3.676	24	1 2 1	24.194
3.487	20	0 3 1	25.528
3.448	11	-1 3 1	25.820
3.226	20	2 0 1	27.632
3.193	26	0 4 0	27.921
3.127	17	2 1 1	28.520
3.089	18	1 3 1	28.878
3.071	33	-1 1 2	29.055
3.038	9	0 0 2	29.378
3.012	10	-2 3 1+	29.639
2.995	16	-3 1 1	29.806
2.957	6	0 1 2	30.195
2.940	11	-2 0 2	30.376
2.879	8	2 2 1	31.041
2.835	22	-1 2 2	31.529
2.776	6	-3 2 1	32.224
2.736	9	3 2 0	32.703
2.602	6	1 4 1	34.438
2.5706	9	2 3 1	34.874
2.5549	9	-2 4 1	35.095
2.5385	3	-1 3 2	35.329
2.4962	23	-3 3 1	35.948
2.4176	4	-2 3 2	37.159
2.4026	1	3 1 1	37.400
2.3571	3	-4 0 1	38.149
2.2852	15	3 2 1	39.399
2.2690	18	2 4 1+	39.692
2.2479	1L	2 0 2+	40.080
2.2355	7	4 1 0	40.312
2.2252	6	2 5 0	40.506
2.2190	6	1 5 1	40.624
2.2006	17	0 4 2	40.980
2.1964	17	3 4 0	41.061
2.1623	4	-2 4 2	41.740
2.1390	5	4 2 0	42.215
2.1213	5	3 3 1	42.585
2.1024	2	-4 1 2	42.986
2.0559	3	-2 1 3	44.008
2.0254	2	0 0 3	44.708
2.0032	11	4 3 0	45.230
1.9657	5	-3 5 1	46.142
1.9518	5	3 5 0	46.490
1.9371	10	-3 1 3	46.863

continued

Ammonium Magnesium Selenate Hydrate, $(NH_4)_2Mg(SeO_4)_2 \cdot 6H_2O$ (continued)

d(A)	I^{rel}	hkl	2θ(°)
1.9237	7	1 6 1	47.210
1.9053	3	-4 3 2	47.694
1.8706	4	-2 3 3	48.636
1.8496	5	4 4 0	49.224
1.8374	4	2 4 2	49.572
1.8294	4	0 3 3	49.804
1.8153	5	-5 2 1+	50.217

Ammonium Magnesium Sulfate Hydrate, $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$

Mineral name
Boussingaultite, syn
Picromerite Group

CAS registry no.
7785-18-4

Sample
The sample was made by evaporation at room temperature of an aqueous solution of $(NH_4)_2SO_4$ and $MgSO_4$.

Color
Colorless

Symmetry classifications

Crystal System	Monoclinic
Space Group	$P2_1/a$ (14)
Pearson Symbol	mP78
Structure Type	A Tutton salt

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	FP Ag
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample
a = 9.3254 (16) Å
b = 12.605 (2)
c = 6.2084 (9)
β = 107.106 (14)°

a/b = 0.7398
c/b = 0.4925

V = 697.49 A^3
Z = 2
Density (calc.) = 1.717 g/cm^3

Figures of merit
F_{30} = 78.7(.0079, 48)
M_{20} = 44.0

Comments
The structure of $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$ was determined by Margulis and Templeton (#1).
The mean temperature of data collection was 22.6°C.

Additional patterns
PDF card 17-135

References
#1. Margulis, T.N. and Templeton, D.H. Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.(1962) 117,334.

d(A)	I^{rel}	hkl	2θ(°)
7.289	2	1 1 0	12.132
6.312	5	0 2 0	14.019
5.942	4	0 0 1	14.896
5.375	55	0 1 1	16.479
5.151	30	1 2 0	17.201
4.456	11	2 0 0	19.909
4.323	26	0 2 1	20.526
4.263	58	-1 2 1	20.819
4.205	100	-2 0 1+	21.109
4.139	31	1 1 1	21.451
3.990	6	-2 1 1	22.263
3.802	85	1 3 0	23.377
3.639	1	2 2 0	24.443
3.597	14	1 2 1	24.728
3.430	18	0 3 1	25.957
3.401	12	-1 3 1	26.184
3.151	54	0 4 0	28.300
3.053	23	2 1 1	29.229
3.012	34	-1 1 2	29.632
2.974	11	-2 3 1+	30.018
2.954	11	-3 1 1	30.233
2.892	17	3 1 0+	30.891
2.816	16	2 2 1	31.756
2.783	34	0 4 1+	32.133
2.738	15	-3 2 1	32.682
2.685	2	0 2 2+	33.339
2.573	7	2 4 0	34.843
2.558	7	1 4 1	35.053
2.519	13	2 3 1	35.618
2.462	22	-3 3 1	36.460
2.4253	4	3 3 0+	37.037
2.3824	3	-2 3 2	37.728
2.3482	1	3 1 1	38.300
2.3226	9	-3 2 2+	38.738
2.2266	13	2 4 1	40.479
2.2100	3	-1 4 2	40.797
2.1937	4	4 1 0+	41.114
2.1873	4	-3 4 1	41.240
2.1788	5	-4 2 1	41.408
2.1614	22	3 4 0	41.758
2.1308	4	-2 4 2	42.385
2.1004	12	4 2 0+	43.030
2.0768	2	3 3 1	43.543
2.0435	2	-2 0 3+	44.289
2.0335	3	-4 3 1	44.520
2.0182	3	-2 1 3	44.874
1.9953	1	-4 2 2	45.420
1.9773	6	0 0 3	45.856
1.9747	6	-1 6 1	45.920
1.9673	4	2 5 1	46.102
1.9570	4	-1 5 2	46.359
1.9408	4	-3 5 1	46.768
1.9219	7	3 5 0	47.256
1.9065	7	-3 1 3	47.663
1.9043	7	3 4 1	47.720

continued

Ammonium Magnesium Sulfate Hydrate, $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$ (continued)

d(Å)	I^{rel}	hkl			2θ(°)
1.9012	6	-2	5	2+	47.804
1.8796	3	-2	6	1	48.387
1.8695	2	-4	4	1	48.665
1.8528	2	-1	3	3	49.133
1.8386	6	-2	3	3	49.537
1.8264	1	3	1	2	49.890
1.8195	4	4	4	0	50.093
1.7983	4	2	4	2	50.727
1.7888	3	-5	2	1	51.015
1.7642	4	5	1	0+	51.779
1.7392	4	-1	6	2	52.579
1.7345	6	3	5	1	52.731
1.7148	4	0	6	2+	53.386
1.6992	1	-2	6	2	53.914

Ammonium Nickel Selenate Hydrate, $(NH_4)_2Ni(SeO_4)_2 \cdot 6H_2O$

Sample

The sample was made by slow evaporation at room temperature of an aqueous solution of $(NH_4)_2SeO_4$ and $NiSeO_4$.

Color

Strong bluish green

Symmetry classifications

Crystal System	Monoclinic
Space Group	$P2_1/a$ (14)
Pearson Symbol	mP78
Structure Type	A Tutton salt

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	FP Ag
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample

a = 9.3283 (14) A
b = 12.6210 (15)
c = 6.3665 (6)
β = 106.23 (1)°

a/b = 0.7391
c/b = 0.5044

V = 719.67 A^3
Z = 2
Density (calc.) = 2.256 g/cm^3

Figures of merit

F_{30} = 90.4(.0079, 42)
M_{20} = 46.2

Comments

The structure of a Tutton salt, $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$, was determined by Margulis and Templeton (#1). The mean temperature of data collection was 23.4°C.

References

#1. Margulis, T.N. and Templeton, D.H. Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.(1962) 117,334.

d(A)	I^{rel}	hkl	2θ(°)
7.312	3	1 1 0	12.095
6.318	7	0 2 0	14.007
6.116	5	0 0 1	14.472
5.503	40	0 1 1	16.092
5.316	6	-1 1 1	16.664
5.158	29	1 2 0	17.177
4.480	18	2 0 0	19.801
4.393	15	0 2 1	20.199
4.298	57	-1 2 1	20.648
4.222	100	-2 1 0+	21.026
4.002	9	-2 1 1	22.197
3.809	68	1 3 0	23.335
3.664	22	1 2 1	24.273
3.466	19	0 3 1	25.679
3.420	16	-1 3 1	26.031
3.211	12	2 0 1	27.761
3.156	15	0 4 0	28.258
3.112	19	2 1 1	28.663
3.080	40	-1 1 2	28.970
2.980	6	-2 3 1+	29.965
2.972	7	0 1 2	30.042
2.954	7	-3 1 1	30.231
2.936	7	-2 0 2	30.425
2.906	3	3 1 0	30.742
2.862	14	2 2 1+	31.232
2.838	13	-1 2 2	31.501
2.781	1	-1 4 1	32.162
2.738	3	-3 2 1	32.680
2.699	8	3 2 0	33.160
2.616	1	1 1 2	34.256
2.582	4	1 4 1	34.709
2.552	5	2 3 1	35.141
2.527	3	-2 4 1	35.496
2.464	28	-3 3 1+	36.440
2.436	2	3 3 0	36.876
2.4066	2	-2 3 2	37.335
2.3853	2	3 1 1	37.682
2.3363	2	-3 2 2	38.502
2.3221	2	-4 0 1	38.747
2.2505	18	2 4 1+	40.031
2.2055	14	4 1 0	40.884
2.1950	20	0 4 2	41.088
2.1686	5	3 4 0	41.613
2.1492	5	-2 4 2	42.006
2.1090	6	-4 0 2+	42.846
2.1036	1L	0 6 0+	42.961
2.0800	1	-4 1 2	43.472
2.0594	3	-2 1 3	43.930
2.0376	3	0 0 3	44.424
2.0089	3	-1 2 3	45.093
1.9796	6	-1 6 1	45.800
1.9411	9	-3 5 1	46.761
1.9338	11	-3 1 3	46.948
1.9275	9	3 5 0	47.110
1.9127	3	4 1 1+	47.499
1.9051	4	1 6 1	47.699
1.8829	4	-2 6 1	48.297
1.8702	4	-2 3 3+	48.647
1.8492	1	4 2 1	49.236
1.8332	7	0 3 3	49.693
1.8260	8	4 4 0	49.904
1.8089	3	3 2 2	50.409
1.7988	2	1 2 3	50.711
1.7886	1	-5 2 1	51.019
1.7734	7	5 1 0+	51.491

continued

d(A)	I^{rel}	hkl			2θ(°)
1.7540	2	-1	6	2+	52.101
1.7412	5	-2	4	3	52.514
1.7197	6	3	6	0	53.223
1.7145	6	1	3	3	53.395
1.7099	6	-2	6	2+	53.550
1.6853	3	2	0	3	54.395
1.6748	6	4	5	0	54.767
1.6492	5	4	4	1	55.690
1.6372	3	-5	3	2	56.132
1.6190	2	-4	5	2	56.821
1.6147	2	-3	6	2	56.988
1.5923	2	4	1	2	57.863
1.5850	3	0	5	3	58.154
1.5680	3	-1	7	2	58.846
1.5531	4	5	2	1+	59.466
1.5470	3	-3	5	3+	59.725

Ammonium Zinc Selenate Hydrate, $(NH_4)_2Zn(SeO_4)_2 \cdot 6H_2O$

Sample

The sample was made by slow evaporation of a 1:1 molar aqueous solution of $(NH_4)_2SeO_4$ and $ZnSeO_4$.

Color

Colorless

Symmetry classifications

Crystal System	Monoclinic
Space Group	$P2_1/a$ (14)
Pearson Symbol	mP78
Structure Type	Tutton salt

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 Å
2θ Standards	Ag FP
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample

a = 9.3806 (13) Å
b = 12.674 (2)
c = 6.3796 (9)
β = 106.226 (12)°

a/b = 0.7401
c/b = 0.5034

V = 728.26 $Å^3$
Z = 2
Density (calc.) = 2.259 g/cm^3

Figures of merit

F_{30} = 73.4(.0100, 41)
M_{20} = 38.8

Comments

The structure of a Tutton salt, $(NH_4)_2Mg(SO_4) \cdot 6H_2O$, was determined by Margulis and Templeton (#1). The mean temperature of data collection was 24.5°C.

Reference

#1. Margulis, T.N., and Templeton, D.H. Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.(1962) 117,334.

d(Å)	I^{rel}	hkl	2θ(°)
7.34	1	1 1 0	12.040
6.334	8	0 2 0	13.971
6.132	8	0 0 1	14.433
5.517	43	0 1 1	16.053
5.180	20	1 2 0	17.104
4.508	19	2 0 0	19.679
4.405	17	0 2 1	20.140
4.312	54	-1 2 1	20.580
4.242	100	2 1 0+	20.923
4.023	9	-2 1 1	22.080
3.826	60	1 3 0	23.230
3.676	23	1 2 1	24.190
3.523	4	-2 2 1	25.260
3.479	18	0 3 1	25.587
3.430	17	-1 3 1	25.956
3.226	8	2 0 1	27.630
3.168	10	0 4 0	28.145
3.123	16	2 1 1	28.561
3.084	43	1 3 1+	28.929
3.064	3	0 0 2	29.120
2.991	5	-2 3 1+	29.853
2.968	5	-3 1 1	30.084
2.944	5	-2 0 2	30.334
2.922	4	3 1 0	30.574
2.874	14	2 2 1	31.098
2.847	15	-1 2 2	31.401
2.791	1	-1 4 1	32.040
2.753	5	-3 2 1	32.497
2.714	7	3 2 0	32.973
2.671	1	-2 2 2	33.530
2.623	3	1 1 2	34.160
2.593	4	1 4 1+	34.560
2.562	6	2 3 1	34.998
2.538	3	-2 4 1	35.332
2.476	27	-3 3 1+	36.259
2.448	2	3 3 0	36.676
2.414	2	-2 3 2	37.218
2.395	2	3 1 1	37.518
2.345	1	-3 2 2	38.347
2.329	1	-1 5 1	38.630
2.259	18	2 4 1	39.873
2.217	9	4 1 0	40.660
2.209	12	2 5 0+	40.816
2.202	16	0 4 2	40.951
2.178	4	3 4 0	41.420
2.1573	5	-2 4 2	41.840
2.1217	6	4 2 0	42.577
2.0892	2	-4 1 2	43.272
2.0644	3	-2 1 3	43.818
2.0408	3	0 0 3	44.351
2.0140	4	-1 2 3	44.974
2.0086	4	-4 2 2	45.102
1.9919	4	2 5 1	45.500
1.9902	4	2 3 2	45.541
1.9504	7	-3 5 1	46.525
1.9446	8	4 0 1+	46.673
1.9391	11	-3 1 3	46.813
1.9328	7	3 4 1	46.974
1.9210	3	-2 5 2	47.279
1.9112	3	2 6 0	47.538
1.8901	4	-2 6 1	48.100
1.8748	4	-3 2 3+	48.518
1.8590	2	4 2 1	48.958
1.8354	10	4 4 0	49.630
1.8163	2	3 2 2	50.187

continued

Ammonium Zinc Selenate Hydrate, $(NH_4)_2Zn(SeO_4)_2 \cdot 6H_2O$ (continued)

d(A)	I^{rel}	hkl			2θ(°)
1.8034	3	1	2	3	50.573
1.7988	2	-5	2	1	50.711
1.7836	6	5	1	0	51.174
1.7598	2	-1	6	2	51.917
1.7460	4	-2	4	3	52.358
1.7366	2	0	7	1+	52.663
1.7324	2	5	2	0	52.801
1.7190	4	-5	2	2+	53.244
1.7141	5	-4	2	3+	53.409
1.6904	2	2	0	3	54.220
1.6841	4	4	5	0	54.439
1.6791	2	2	7	0	54.614
1.6564	2	5	3	0	55.426

Ammonium Zinc Sulfate Hydrate, $(NH_4)_2Zn(SO_4)_2 \cdot 6H_2O$

CAS registry no.
7783-24-6

Sample
The sample was made by slow evaporation at room temperature of an aqueous solution of $(NH_4)_2SO_4$ and $ZnSO_4$.

Color
Colorless

Symmetry classifications

Crystal System	Monoclinic
Space Group	$P2_1/a$ (14)
Pearson Symbol	mP78
Structure Type	A Tutton salt

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	Ag FP
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±3

Crystallographic constants of this sample

a = 9.2388 (12) Å
b = 12.5173 (16)
c = 6.2516 (8)
β = 106.852 (11)°

a/b = 0.7381
c/b = 0.4994

V = 691.92 A^3
Z = 2
Density (calc.) = 1.928 g/cm^3

Figures of merit
F_{30} = 142.9(.0060, 35)
M_{20} = 82.9

Comments
The structure of a Tutton salt, $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$, was determined by Margulis and Templeton (#1).
The mean temperature of data collection was 23.4°C.

Additional patterns
PDF card 18-138

References
#1. Margulis, T.N. and Templeton, D.H. Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.(1962) 117,334.

d(A)	I^{rel}	hkl			2θ(°)
7.228	3	1	1	0	12.235
6.258	14	0	2	0	14.142
5.983	15	0	0	1	14.795
5.400	31	0	1	1	16.401
5.262	9	-1	1	1	16.837
5.111	12	1	2	0	17.338
4.421	21	2	0	0	20.067
4.325	23	0	2	1	20.520
4.254	36	-1	2	1	20.864
4.182	100	-2	0	1	21.230
4.148	61	1	1	1	21.404
3.967	6	-2	1	1	22.396
3.774	77	1	3	0	23.553
3.611	12	2	2	0	24.637
3.599	16	1	2	1	24.720
3.476	5	-2	2	1	25.608
3.423	16	0	3	1	26.010
3.386	20	-1	3	1	26.296
3.146	12	2	0	1	28.344
3.126	12	0	4	0	28.527
3.051	34	2	1	1	29.245
3.037	48	2	3	0	29.390
3.030	50	-1	1	2	29.453
2.954	4	-2	3	1	30.236
2.928	5	-3	1	1	30.511
2.910	7	0	1	2	30.701
2.898	7	-2	0	2	30.828
2.870	7	3	1	0	31.143
2.811	30	2	2	1	31.804
2.793	25	-1	2	2	32.018
2.7541	1	-1	4	1	32.484
2.7147	9	-3	2	1	32.968
2.6664	1	3	2	0	33.583
2.6288	2	-2	2	2	34.078
2.5555	12	2	4	0	35.087
2.5116	7	2	3	1	35.721
2.4430	29	-3	3	1+	36.759
2.4085	4	1	5	0+	37.304
2.3802	2	-2	3	2	37.765
2.3420	5	3	1	1	38.405
2.3084	2	0	5	1	38.986
2.3014	1	-4	0	1	39.109
2.2644	1	-4	1	1	39.776
2.2177	17	2	4	1	40.649
2.1765	8	4	1	0+	41.455
2.1702	11	-3	4	1	41.579
2.1623	12	0	4	2	41.740
2.1470	8	-2	5	1	42.051
2.1394	8	-3	3	2	42.207
2.1260	6	-2	4	2	42.487
2.0838	12	4	2	0	43.390
2.0545	1	-2	0	3	44.040
2.0273	14	-2	1	3	44.662
1.9949	5	0	0	3	45.429
1.9837	4	-4	2	2	45.700

continued

Ammonium Zinc Sulfate Hydrate, $(NH_4)_2Zn(SO_4)_2 \cdot 6H_2O$ (continued)

d(A)	I^{rel}	hkl			2θ(°)
1.9699	4	0	6	1+	46.038
1.9594	3	2	5	1	46.299
1.9535	2	4	3	0+	46.447
1.9260	6	-3	5	1	47.151
1.9206	6	0	5	2	47.290
1.9091	13	-3	1	3+	47.594
1.8868	2	2	6	0	48.190
1.8665	6	-2	6	1	48.748
1.8611	6	-1	3	3	48.900
1.8436	4	-2	3	3	49.393
1.8281	4	-5	1	1	49.841
1.8198	4	4	2	1	50.085
1.8151	5	1	1	3	50.223
1.8078	6	1	5	2	50.440
1.7993	7	2	4	2+	50.696

Antimony Phosphate, $SbPO_4$

Synonym
Antimony orthophosphate

CAS registry no.
14713-43-0

Sample
The sample was made by stirring Sb_2O_3 in an excess of 6 M H_3PO_4 for 5 days.

Color
Colorless

Symmetry classifications

Crystal System	Monoclinic
Space Group	$P2_1/m$ (11)
Pearson Symbol	mP12

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample
a = 5.1057 (7) A
b = 6.7724 (7)
c = 4.7454 (4)
β = 94.613 (9)°

a/b = 0.7539
c/b = 0.7007

V = 163.55 A^3
Z = 2
Density (calc.) = 4.401 g/cm^3

Figures of merit
F_{30} = 104.7(.0077, 37)
M_{20} = 89.1

Comments
The structure of $SbPO_4$ was determined by Kinberger (#1).
The mean temperature of data collection was 24.4°C.

Additional patterns
PDF card 23-793
Majling et al. (#2)

References

#1. Kinberger, B.
Acta Chem. Scand.(1970) 24,320.
#2. Majling, J. et al.; (1979)
Calculated Powder Diffraction Patterns for Anhydrous Phosphates (VEDA, Bratislava, Czechoslovakia).

d(A)	I^{rel}	hkl	2θ(°)
4.734	8	0 0 1	18.731
4.066	60	1 1 0	21.840
3.876	33	0 1 1	22.925
3.611	100	-1 0 1	24.637
3.386	92	0 2 0	26.299
3.334	36	1 0 1	26.719
3.189	5	-1 1 1	27.956
2.992	51	1 1 1	29.834
2.545	14	2 0 0	35.236
2.471	35	-1 2 1	36.332
2.3832	44	2 1 0	37.716
2.3756	36	1 2 1	37.840
2.3650	30	0 0 2	38.017
2.3205	1	-2 0 1	38.775
2.2329	2	0 1 2	40.360
2.2137	2	-1 0 2	40.727
2.1949	6	-2 1 1	41.091
2.1700	15	2 0 1	41.584
2.1046	21	-1 1 2	42.940
2.0816	7	1 0 2	43.438
2.0638	30	1 3 0	43.831
2.0374	22	0 3 1	44.429
1.9903	2	1 1 2	45.538
1.9390	17	0 2 2	46.815
1.9151	3	-1 3 1	47.434
1.8694	19	1 3 1	48.667
1.8266	9	2 2 1	49.885
1.8061	12	-2 0 2	50.492
1.7731	1	1 2 2	51.500
1.7447	2	-2 1 2	52.400
1.6931	20	0 4 0	54.124
1.6887	18	2 3 0	54.278
1.6456	3	3 1 0	55.820
1.6333	4	0 3 2	56.280
1.6179	16	-2 3 1+	56.864
1.5938	22	-2 2 2+	57.804
1.5806	11	-1 3 2	58.332
1.5766	7	0 0 3	58.494
1.5645	4	2 3 1	58.990
1.5415	6	-1 0 3	59.960
1.5331	10	-1 4 1	60.323
1.5177	10	3 1 1	61.001
1.5093	4	1 4 1	61.379
1.4732	1L	1 0 3	63.050
1.4390	8	1 1 3	64.731
1.4297	2	0 2 3	65.200
1.4099	2	2 4 0+	66.235
1.4026	10	-1 2 3+	66.624
1.3913	1L	-2 0 3	67.236
1.3763	5	0 4 2	68.067
1.3625	3	-2 1 3	68.857
1.3406	5	2 3 2	70.140
1.3344	3	2 4 1	70.517
1.3264	5	-3 3 1	71.007
1.3092	1	1 5 0	72.086

continued

Antimony Phosphate, $SbPO_4$ (continued)

d(A)	I^{rel}	hkl			2θ(°)
1.2945	1L	2	0	3	73.036
1.2817	5	3	3	1	73.885
1.2545	4	1	5	1+	75.761
1.2353	4	-2	4	2	77.156
1.2334	6	-4	1	1+	77.297
1.2108	1	-3	3	2	79.016

Barium Bismuth Titanium Oxide, $BaBi_4Ti_4O_{15}$

Synonym
Barium bismuth titanate

Sample
The sample was prepared in the early 1960's by W.S. Brower at NBS. The starting materials $BaCO_3$, Bi_2O_3, and TiO_2 (anatase) were heated in a platinum crucible to about 700°C, then calcined at about 1000°C.

Color
Colorless

Symmetry classifications

Crystal System	Tetragonal
Space Group	I4/mmm (139)
Pearson Symbol	tI48

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	W FP
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±1

Crystallographic constants of this sample
a = 3.8624 (3) A
c = 41.851 (4)

c/a = 10.8355

V = 624.34 A^3
Z = 2
Density (calc.) = 7.473 g/cm^3

Figures of merit
F_{30} = 86.1(.0077, 45)
M_{20} = 81.2

Comments
The structure was determined by Aurivillius (#1).
The mean temperature of data collection was 24.7°C.

Additional patterns
PDF card 8-261

Reference
#1. Aurivillius, B.
Ark. Kemi(1951) 2,519.

d(A)	I^{rel}	hkl	2θ(°)
10.47	2	0 0 4	8.439
6.977	3	0 0 6	12.677
5.233	9	0 0 8	16.930
4.186	7	0 0 10	21.210
3.846	18	1 0 1	23.107
3.722	2	1 0 3	23.886
3.504	2	1 0 5	25.395
3.243	6	1 0 7	27.479
2.970	100	1 0 9	30.061
2.730	36	1 1 0	32.775
2.643	1	1 1 4	33.896
2.615	2	0 0 16	34.258
2.543	1	1 1 6	35.267
2.473	1	1 0 13	36.297
2.4202	4	1 1 8	37.118
2.3244	8	0 0 18	38.707
2.2869	20	1 1 10	39.368
2.2621	2	1 0 15	39.817
2.0921	2	0 0 20	43.209
2.0752	4	1 0 17	43.579
2.0155	1	1 1 14	44.939
1.9315	22	2 0 0	47.008
1.9135	6	1 0 19	47.478
1.8887	4	1 1 16	48.138
1.8119	2	2 0 8	50.318
1.7706	16	1 1 18+	51.577
1.7538	2	2 0 10	52.107
1.7260	4	2 1 1	53.011
1.6893	1	2 0 12	54.257
1.6600	2	2 1 7	55.295
1.6463	1L	1 0 23	55.796
1.6194	21	2 1 9	56.806
1.5537	2	2 0 16	59.441
1.5365	2	1 0 25	60.176
1.4949	1	0 0 28	62.034
1.4854	5	2 0 18	62.472
1.4694	1	1 1 24	63.234
1.4387	5	1 0 27	64.742
1.4192	1	2 0 20	65.744
1.4139	1	2 1 17	66.024

Barium Copper Phosphate, $Ba_2Cu(PO_3)_6$

Synonym
Barium copper metaphosphate

Sample
A 1:4:12 molar mixture of $CuCo_3 \cdot Cu(OH)_2$, $BaCO_3$, and $NH_4H_2PO_4$ was heated up to 500°C, reground and heated at 800°C for 40 hours.

Color
Very pale green

Symmetry classifications

Crystal System	Monoclinic
Space Group	$P2_1/a$ (14)
Pearson Symbol	mP108

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample
a = 21.410 (2) A
b = 7.2792 (9)
c = 9.5221 (12)
β = 97.945 (12)°

a/b = 2.9413
c/b = 1.3081

V = 1469.75 A^3
Z = 4
Density (calc.) = 3.670 g/cm^3

Figures of merit
F_{30} = 91.9(.0076, 43)
M_{20} = 34.1

Comments
The structure was determined by Laugt and Guitel (#1).
The mean temperature of data collection was 24.5°C.

Additional patterns
PDF card 25-65
Majling et al. (#2)

References

#1. Laugt, M. and Guitel, J.-C. Acta Crystallogr.(1975) B31,1148.
#2. Majling, J. et al.; (1979) Calculated Powder Diffraction Patterns for Anhydrous Phosphates (VEDA, Bratislava, Czechoslovakia).

d(A)	I^{rel}	hkl	2θ(°)
10.61	3	2 0 0	8.329
7.583	5	-2 0 1	11.660
6.602	4	2 0 1	13.400
5.994	3	2 1 0	14.768
5.678	3	-1 1 1	15.595
5.299	3	4 0 0	16.716
5.249	4	-2 1 1	16.876
5.069	9	3 1 0	17.480
4.919	9	-4 0 1	18.017
4.892	7	2 1 1	18.120
4.714	2	0 0 2	18.810
4.665	3	-3 1 1	19.009
4.368	5	4 0 1	20.315
4.296	3	3 1 1	20.660
4.284	5	4 1 0	20.719
4.101	33	2 0 2	21.650
4.073	25	-4 1 1	21.801
3.976	7	-1 1 2	22.344
3.957	9	0 1 2	22.448
3.856	5	-2 1 2	23.049
3.793	35	-4 0 2	23.437
3.746	9	4 1 1	23.734
3.663	20	5 1 0	24.276
3.637	25	-3 1 2+	24.454
3.574	15	2 1 2	24.895
3.533	12	6 0 0	25.190
3.395	6	0 2 1	26.230
3.364	23	-4 1 2	26.471
3.327	100	1 2 1	26.777
3.303	29	4 0 2	26.973
3.282	13	-2 2 1	27.150
3.236	9	3 2 0	27.540
3.189	8	2 2 1	27.960
3.178	11	6 1 0	28.054
3.133	7	-6 1 1+	28.470
3.077	1	-5 1 2	29.000
3.037	29	-6 0 2	29.387
3.002	15	3 2 1+	29.736
2.927	4	-4 2 1	30.518
2.909	10	-1 1 3+	30.715
2.884	20	-4 0 3+	30.984
2.841	4	-2 2 2	31.460
2.823	5	1 2 2	31.664
2.813	8	1 1 3	31.788
2.799	11	-3 1 3+	31.949
2.779	4	-7 1 1	32.183
2.740	11	5 1 2	32.661
2.717	5	-5 2 1	32.939
2.682	1	-4 1 3	33.385
2.650	21	8 0 0+	33.795
2.593	17	7 1 1+	34.569
2.561	8	3 1 3	35.005
2.553	6	4 0 3+	35.116
2.483	11	-5 2 2	36.147
2.4608	7	-8 0 2	36.483

continued

Barium Copper Phosphate, $Ba_2Cu(PO_3)_6$ (continued)

d(Å)	I^{rel}	hkl			2θ(°)
2.4113	2	1	3	0+	37.260
2.3726	9	-2	0	4	37.891
2.3655	4	2	3	0	38.008
2.3367	6	1	2	3	38.496
2.3304	10	-8	1	2+	38.604
2.3192	20	-7	2	1	38.798
2.3124	13	-2	3	1	38.917
2.2949	8	3	3	0+	39.225
2.2814	8	7	1	2	39.467
2.2747	8	-4	0	4	39.588
2.2558	3	-2	1	4+	39.933
2.2496	2	-9	1	1	40.048
2.2434	3	0	1	4+	40.163
2.2365	3	2	0	4+	40.293
2.2014	13	1	1	4+	40.965
2.1865	5	3	2	3+	41.255
2.1757	12	-4	3	1+	41.471
2.1605	7	-1	3	2	41.775
2.1328	13	-10	0	1+	42.343
2.1199	4	10	0	0+	42.615
2.1068	8	5	3	0+	42.892
2.1009	11	-3	3	2+	43.019
2.0940	8	8	1	2	43.168
2.0879	8	2	3	2+	43.299
2.0408	5	8	2	1	44.352
2.0274	3	3	3	2	44.661
1.9877	6	5	2	3+	45.602
1.9822	5	-9	2	1	45.736
1.9741	11	-5	3	2+	45.935
1.9658	9	-3	2	4+	46.138
1.9275	5	-1	3	3+	47.111
1.9202	6	0	3	3	47.301
1.9032	6	-2	0	5	47.750
1.8984	5	1	3	3	47.878
1.8920	7	9	2	1	48.049
1.8469	2	6	0	4	49.301
1.8410	2	-2	1	5+	49.469
1.8264	6	7	3	1+	49.890
1.8178	10	-11	1	2+	50.142
1.8137	5	1	4	0+	50.266
1.7847	4	10	1	2+	51.139
1.7428	2	-9	1	4+	52.463
1.7304	2	-12	1	1	52.867
1.7181	3	5	2	4+	53.276
1.7134	3	-11	2	1+	53.433
1.7032	7	11	2	0+	53.780
1.6984	5	7	1	4+	53.941
1.6949	4	12	0	1	54.063
1.6907	3	0	3	4+	54.209
1.6758	3	-3	2	5	54.729
1.6719	3	-10	2	3+	54.869
1.6637	1	2	4	2	55.162

Barium Silicate, $Ba_5Si_8O_{21}$

Synonym
Barium silicon oxide

CAS registry no.
11092-02-7

Sample
Stoichiometric amounts of $BaCO_3$ and SiO_2 were ground together and heated to 900°C for 20 hours, 1300°C for 22.5 hours, and 1375°C for 21.5 hours with intermittent grinding. Silicon oxide, SiO_2 (0.4 mol. %) was added for a final heating at 1375°C for 22.5 hours.

Color
Colorless

Symmetry classifications
Crystal System Monoclinic
Space Group I*/a
Pearson Symbol mC136

Data collection and analysis parameters
Radiation $CuK\alpha_1$
Wavelength 1.5405981 A
2θ Standards Si FP
Scanned to 5.0° 2θ
$\sigma(I^{rel})$ ±6

Crystallographic constants of this sample
a = 32.697 (4) A
b = 4.6977 (9)
c = 13.901 (2)
β = 98.144 (10)°

a/b = 6.9602
c/b = 2.9591

V = 2113.67 A^3
Z = 4
Density (calc.) = 3.920 g/cm^3

Figures of merit
F_{30} = 72.1(.0083, 50)
M_{20} = 38.5

Comments
The unit cell was determined by Roth (#1).
The mean temperature of data collection was 24.0°C.

Additional patterns
PDF card 12-548

Reference
#1. Roth, R.S.
Priv. Commun.(1966)

d(A)	I^{rel}	hkl			2θ(°)
16.27	1L	2	0	0	5.426
8.10	1L	4	0	0	10.911
6.881	13	0	0	2	12.855
6.684	1	-2	0	2	13.236
6.031	10	2	0	2	14.677
5.657	1	-4	0	2	15.651
5.396	1	6	0	0	16.413
4.911	1L	4	0	2	18.048
4.344	2	-2	1	1	20.427
4.307	8	3	1	0	20.607
4.241	2	2	1	1	20.928
4.046	1	8	0	0	21.949
3.890	10	-1	1	2	22.841
3.801	100	5	1	0	23.387
3.726	74	-8	0	2	23.861
3.560	4	3	1	2	24.989
3.509	1	-6	1	1	25.362
3.467	3	-2	0	4	25.675
3.439	3	0	0	4	25.884
3.341	7	-4	0	4	26.661
3.289	51	8	0	2	27.087
3.272	82	2	0	4	27.231
3.237	42	10	0	0	27.533
3.218	62	5	1	2	27.703
3.107	31	-6	0	4	28.706
3.015	1L	4	0	4	29.605
2.939	2	-6	1	3+	30.388
2.860	11	7	1	2	31.250
2.854	9	9	1	0	31.316
2.826	20	-8	0	4	31.635
2.781	61	10	0	2	32.159
2.765	42	-3	1	4	32.355
2.740	3	1	1	4	32.659
2.697	2	12	0	0	33.191
2.677	5	-10	1	1	33.440
2.665	6	-5	1	4	33.597
2.617	2	3	1	4	34.237
2.543	3	-10	0	4	35.258
2.537	3	9	1	2	35.354
2.509	3	-7	1	4	35.761
2.440	3	-11	1	2	36.802
2.399	1	12	0	2	37.465
2.392	1L	-2	1	5	37.579
2.374	3	0	1	5	37.869
2.3486	39	0	2	0	38.292
2.3298	2	-9	1	4	38.613
2.3117	2	14	0	0+	38.929
2.3052	2	1	2	1	39.042
2.2926	5	-14	0	2+	39.266
2.2858	6	-12	0	4	39.387
2.2677	40	7	1	4	39.716
2.2272	26	-6	0	6+	40.469
2.2003	21	13	1	0	40.985
2.1947	15	-12	1	3+	41.095
2.1761	49	-13	1	2	41.462

continued

d(A)	I^{rel}	hkl			2θ(°)
2.1461	18	-11	1	4	42.069
2.1286	4	-8	0	6+	42.431
2.0850	5	9	1	4	43.362
2.0736	17	-3	1	6+	43.613
2.0407	4	1	1	6+	44.353
2.0281	4	-5	2	3+	44.643
2.0200	4	-16	0	2	44.834
2.0102	1	-10	0	6+	45.064
1.9909	23	12	0	4	45.524
1.9680	2	-9	2	1+	46.084
1.9607	5	15	1	0	46.267
1.9542	6	-15	1	2+	46.429
1.9083	15	2	2	4	47.613
1.9005	7	10	2	0+	47.821
1.8957	3	5	1	6+	47.951
1.8840	2	8	0	6+	48.266
1.8739	10	-16	1	1+	48.543
1.8628	5	-16	0	4	48.853
1.8248	16	15	1	2	49.939
1.8061	14	14	1	3+	50.492
1.7985	52	18	0	0+	50.719
1.7773	2	2	1	7	51.368
1.7677	2	-14	1	5	51.669
1.7651	2	17	1	0+	51.749
1.7572	8	-14	0	6+	51.999
1.7333	7	-4	0	8	52.770
1.7104	2	-6	0	8	53.535
1.6975	2	9	1	6+	53.972
1.6576	2	17	1	2	55.382
1.6380	24	-12	2	4	56.103
1.6237	11	-1	1	8	56.642
1.6160	20	-6	2	6+	56.937
1.6077	2	-19	1	2+	57.259
1.6030	2	1	1	8	57.440
1.5950	1	-15	1	6+	57.755
1.5771	1	-8	2	6+	58.475
1.5671	1L	14	2	2+	58.886
1.5527	10	-9	1	8+	59.486

Barium Titanium Borate, $BaTi(BO_3)_2$

Synonym

Barium titanium bis(borate)

Sample

The sample was prepared by J.M. Millet by heating stoichiometric amounts of $BaTiO_3$ and H_3BO_3 at 700°C for 2 hours. Then it was ground and heated for 2 successive periods at 950°C for 24 hours.

Color

Colorless

Symmetry classifications

Crystal System	Rhombohedral
Space Group	$R\bar{3}$(148)
Pearson Symbol	hR10
Structure Type	Dolomite

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Ag
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample

Hexagonal axes)

a = 5.02331 (16) A

c = 16.3939 (7)

c/a = 3.2636

V = 358.26 A^3

Z = 3

Density (calc.) = 4.211 g/cm^3

Figures of merit

F_{30} = 151.5(.0060, 33)

M_{20} = 245.4

Comments

The structure was studied by Vicat and Aléonard (#1). The temperature of data collection was approximately 25.0°C.

Additional patterns

PDF card 22-96

Reference

#1. Vicat, J. and Aléonard, S. C. R. Seances Acad. Sci., Ser. C(1968) 266,1046.

d(A)	I^{rel}	hkl	2θ(°)
5.465	7	0 0 3	16.206
4.204	19	1 0 1	21.114
3.843	73	0 1 2	23.126
2.984	100	1 0 4	29.925
2.7316	4	0 0 6	32.759
2.6193	22	0 1 5	34.205
2.5118	35	1 1 0	35.718
2.2825	15	1 1 3	39.447
2.1565	19	0 2 1	41.856
2.1025	29	2 0 2	42.985
2.0624	5	1 0 7	43.862
1.9214	9	0 2 4	47.270
1.8542	36	0 1 8	49.092
1.8493	45	1 1 6	49.233
1.8217	5	0 0 9	50.030
1.6359	2	2 1 1	56.183
1.6122	16	1 2 2	57.084
1.5341	7	1 0 10	60.280
1.5260	17	2 1 4	60.634
1.4915	7	2 0 8	62.190
1.4742	5	1 1 9	63.001
1.4701	6	1 2 5	63.198
1.4502	6	3 0 0	64.167
1.4100	1L	0 1 11	66.229
1.4015	3	3 0 3	66.680
1.3661	2	0 0 12	68.647
1.3455	2	2 1 7	69.852
1.3089	8	0 2 10	72.102
1.2827	9	1 2 8	73.816
1.2809	10	3 0 6	73.939
1.2558	6	2 2 0	75.669
1.2293	1L	2 0 11	77.601
1.2238	1L	2 2 3	78.015
1.2113	1L	1 0 13	78.980
1.2034	3	1 3 1	79.600
1.2001	7	1 1 12	79.863
1.1935	5	3 1 2	80.391
1.1609	4	2 1 10	83.137
1.1577	9	1 3 4	83.424
1.1410	3	2 2 6	84.928
1.1346	2	3 0 9	85.519
1.1324	8	3 1 5	85.728
1.1306	2	0 1 14	85.894
1.1044	1L	1 2 11	88.449
1.0909	1L	0 2 13	89.840
1.0852	1L	4 0 1	90.440
1.0781	1L	0 4 2	91.201
1.0726	1L	1 3 7	91.808
1.0511	2	4 0 4	94.251
1.03976	5	3 1 8	95.607
1.03382	1L	2 2 9	96.335
1.03119	1L	2 0 14	96.662
1.00220	1L	1 1 15	100.458

Barium Titanium Oxide, $BaTi_5O_{11}$

Synonym
Barium titanate

Sample
The sample was prepared at NBS by J. J. Ritter by hydrolysis of a nonaqueous solution containing barium and titanium ethoxides in a 1:5 molar ratio. The precipitate was recovered and dried at 110°C. The sample was then heated at 1100°C for 22 hours.

Color
Colorless

Symmetry classifications
Crystal System Monoclinic
Space Group $P2_1/n$ (14)
Pearson Symbol mP68

Data collection and analysis parameters
Radiation $CuK\alpha_1$
Wavelength 1.5405981 A
2θ Standard W
Scanned to 5.0° 2θ
$\sigma(I^{rel})$ ±3

Crystallographic constants of this sample
a = 7.6691 (4) A
b = 14.0410 (8)
c = 7.5335 (5)
β = 98.359 (5)°

a/b = 0.5462
c/b = 0.5365

V = 802.64 A^3
Z = 4
Density (calc.) = 4.575 g/cm^3

Figures of merit
F_{30} = 92.6(.0061, 53)
M_{20} = 45.2

Comments
The structure was determined by Tillmanns (#1).
The mean temperature of data collection was 23.4°C.

Additional patterns
PDF card 29-205

Reference
#1. Tillmanns, E.
Acta Crystallogr., Sect. B(1969) 25, 1444.

d(A)	I^{rel}	hkl	2θ(°)
6.683	4	1 1 0	13.238
5.757	6	-1 0 1	15.380
5.159	9	1 2 0	17.174
4.970	4	1 0 1	17.834
4.684	2	1 1 1	18.932
3.966	24	0 3 1	22.398
3.796	38	2 0 0	23.415
3.729	31	0 0 2	23.843
3.511	15	0 4 0	25.346
3.447	31	-1 1 2	25.823
3.408	3	1 3 1	26.126
3.338	29	2 2 0	26.685
3.292	26	0 2 2	27.062
3.203	27	-2 2 1	27.831
3.187	74	1 4 0	27.974
3.176	100	0 4 1	28.076
3.119	11	2 1 1	28.600
3.090	13	1 1 2	28.870
2.997	18	-1 4 1	29.790
2.911	80	2 2 1	30.693
2.888	28	1 2 2	30.943
2.876	29	-2 0 2	31.068
2.867	28	1 4 1	31.169
2.832	30	-1 3 2	31.571
2.661	12	-2 2 2	33.651
2.640	9	2 3 1	33.929
2.628	9	0 5 1	34.090
2.5136	35	-2 4 1	35.691
2.5081	34	-3 0 1	35.772
2.4893	1	3 1 0	36.052
2.4847	3	2 0 2	36.121
2.4696	7	-3 1 1+	36.349
2.4465	13	0 1 3+	36.705
2.4326	4	-1 1 3	36.921
2.3795	5	3 2 0	37.776
2.3625	5	-3 2 1+	38.058
2.3420	9	0 2 3+	38.404
2.3294	6	-1 2 3	38.621
2.2657	3	1 0 3+	39.751
2.2429	6	0 5 2	40.173
2.2370	8	1 1 3+	40.283
2.2320	6	0 6 1	40.378
2.2112	17	-3 3 1	40.774
2.2050	17	-2 1 3+	40.894
2.1942	33	2 3 2+	41.104
2.1840	23	-1 3 3	41.306
2.1677	18	-1 6 1	41.630
2.1429	6	-3 2 2	42.134
2.1276	7	-2 2 3	42.452
2.1171	14	1 6 1	42.673
2.0613	2	3 3 1	43.888
2.0521	27	3 4 0	44.094
2.0410	37	-3 4 1	44.347
2.0279	27	0 4 3+	44.649
2.0200	25	-1 4 3	44.834

continued

d(A)	I^{rel}	hkl	2θ(°)
2.0146	10	-2 3 3	44.960
1.9918	4	2 6 0	45.502
1.9820	4	0 6 2	45.740
1.9545	5	-1 6 2	46.421
1.9453	6	3 1 2	46.654
1.9339	8	2 1 3	46.946
1.9213	5	3 4 1	47.273
1.9165	4	-3 0 3	47.397
1.9034	6	1 4 3	47.743
1.8939	8	-1 7 1+	47.999
1.8838	8	-2 4 3	48.272
1.8709	8	-3 5 1	48.627
1.8608	25	0 5 3+	48.909
1.8548	28	-1 5 3	49.075
1.8499	9	-3 2 3	49.214
1.8390	3	-4 2 1	49.526
1.8312	4	4 2 0	49.751
1.8154	3	-2 6 2	50.215
1.7998	7	-4 0 2	50.679
1.7777	3	-2 0 4+	51.356
1.7741	3	-3 3 3+	51.467
1.7645	5	-4 3 1+	51.769
1.7557	8	-3 5 2+	52.046
1.7429	5	-4 2 2	52.460
1.7386	2	1 1 4	52.598
1.7309	4	0 3 4	52.851
1.7231	6	4 2 1+	53.108
1.7098	14	1 8 0	53.553
1.7032	14	2 6 2+	53.777
1.6989	11	-1 6 3+	53.925
1.6825	4	-3 4 3	54.494
1.6786	4	-1 8 1	54.632
1.6746	4	-4 4 1	54.774
1.6620	3	-2 3 4+	55.223
1.6547	3	1 8 1	55.490
1.6391	14	3 6 1	56.061
1.6278	4	1 6 3	56.488
1.6151	5	-4 1 3+	56.970
1.6060	3	-3 1 4	57.322
1.6032	3	2 5 3	57.432
1.5989	2	4 0 2	57.600
1.5886	3	4 1 2	58.010
1.5853	3	4 4 1+	58.142
1.5779	5	-2 8 1+	58.443
1.5736	5	-1 8 2+	58.616
1.5667	5	-3 7 1+	58.899
1.5607	17	0 7 3+	59.150
1.5569	17	-1 7 3	59.307
1.5359	5	-4 3 3+	60.204
1.5281	4	-3 3 4+	60.544
1.5131	2	4 3 2	61.205
1.5058	2	-1 9 1	61.535
1.5001	5	2 3 4	61.792
1.4973	5	-3 7 2+	61.923
1.4862	9	1 5 4	62.436

d(A)	I^{rel}	hkl	2θ(°)
1.4830	15	-3 6 3+	62.588
1.4753	4	-4 4 3	62.951
1.4684	2	-3 4 4	63.282
1.4538	4	-2 1 5	63.989
1.4508	6	-5 2 2	64.137
1.4466	8	5 0 1	64.349
1.4422	10	3 8 0	64.569
1.4380	20	-3 8 1+	64.777
1.4308	6	-2 2 5+	65.143
1.4284	2	-1 9 2	65.267
1.4240	5	1 0 5	65.494
1.4167	4	5 2 1+	65.875

Barium Titanium Oxide, Ba_2TiO_4

Synonym
Barium orthotitanate

CAS registry no.
12009-63-1

Sample
Ba_2TiO_4 was prepared by grinding $BaTiO_3$ and $BaCO_3$ together and heating the mixture to 800°C for 19 hours, 1000°C for 140 hours, 1525°C for 37 hours, and 1480°C for 24 hours (#1).

Color
Yellowish gray

Symmetry classifications

Crystal System	Monoclinic
Space Group	$P2_1/n$ (14)
Pearson Symbol	mP28

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	W FP
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±5

Crystallographic constants of this sample

a = 10.5496 (7) A
b = 7.6735 (6)
c = 6.1147 (5)
β = 93.182 (6)°

a/b = 1.3748
c/b = 0.7969

V = 494.24 A^3
Z = 4
Density (calc.) = 5.195 g/cm^3

Figures of merit
F_{30} = 77.5(.0082, 47)
M_{20} = 49.4

Comments
The structure was determined by Bland (#1).
The mean temperature of data collection was 24.8°C.

Additional patterns
PDF card 8-277

Reference
#1. Bland, J.A.
Acta Crystallogr.(1961) 14,875.

d(A)	I^{rel}	hkl	2θ(°)
5.418	7	-1 0 1	16.347
5.158	1	1 0 1	17.179
4.423	8	-1 1 1	20.061
4.345	5	2 1 0	20.425
4.282	4	1 1 1	20.727
3.619	24	-2 1 1	24.582
3.465	33	2 1 1	25.688
3.249	33	0 2 1	27.432
3.193	25	3 1 0	27.924
3.132	29	-1 2 1	28.473
3.121	100	-3 0 1	28.576
3.101	52	2 2 0	28.765
3.079	50	1 2 1	28.974
3.052	69	0 0 2	29.242
2.975	50	3 0 1	30.015
2.836	8	0 1 2	31.516
2.801	8	-2 2 1	31.926
2.774	5	-1 1 2+	32.240
2.729	9	2 2 1	32.786
2.706	4	-2 0 2+	33.072
2.633	7	4 0 0	34.028
2.591	26	3 2 0	34.590
2.553	5	-2 1 2	35.124
2.492	36	4 1 0	36.010
2.445	12	2 1 2	36.720
2.390	6	0 2 2	37.607
2.3514	10	-1 2 2+	38.246
2.3085	12	1 2 2	38.985
2.3020	11	2 3 0	39.100
2.2642	21	-3 1 2+	39.779
2.2113	25	-2 2 2	40.772
2.1705	7	-2 3 1+	41.574
2.1526	16	3 1 2	41.937
2.1409	15	2 2 2	42.175
2.0676	8	3 3 0	43.746
2.0313	26	5 1 0	44.569
2.0261	21	-5 0 1	44.690
2.0160	16	-3 2 2+	44.926
1.9671	3	0 1 3	46.106
1.9580	6	5 0 1+	46.334
1.9527	5	-1 1 3	46.467
1.9400	20	-1 3 2+	46.789
1.9357	19	3 2 2	46.898
1.9152	13	1 1 3+	47.432
1.8820	3	4 1 2	48.322
1.8466	6	5 2 0	49.309
1.8306	8	0 4 1	49.770
1.8116	23	2 1 3	50.328
1.8046	27	-3 0 3	50.537
1.7979	22	0 2 3+	50.739
1.7871	14	-1 2 3	51.065
1.7761	19	-4 3 1	51.407
1.7557	11	6 0 0	52.046
1.7391	22	4 3 1+	52.582
1.7348	19	-5 1 2	52.724

continued

Barium Titanium Oxide, Ba_2TiO_4 (continued)

d(A)	I^{rel}	hkl			2θ(°)
1.7199	11	2	4	1+	53.214
1.6864	11	3	3	2	54.358
1.6835	10	3	4	0	54.458
1.6712	8	-6	1	1	54.893
1.6510	12	5	1	2	55.624
1.6249	8	6	1	1+	56.595
1.6152	5	-5	2	2	56.968
1.5966	8	6	2	0	57.693
1.5925	4	0	3	3	57.854
1.5652	10	-2	4	2+	58.964
1.5598	10	-6	0	2	59.186
1.5468	3	5	2	2+	59.735
1.5369	5	4	1	3	60.159
1.5263	16	0	0	4+	60.619
1.4911	2	-3	4	2+	62.209
1.4866	5	6	0	2	62.416
1.4765	2	-1	5	1+	62.893
1.4734	2	2	5	0	63.041
1.4716	3	1	5	1+	63.129
1.4575	7	3	4	2	63.809
1.4451	3	-6	2	2+	64.422
1.4423	7	7	0	1	64.561
1.4276	1L	2	5	1+	65.311
1.4060	2	3	5	0	66.442
1.4012	3	-4	4	2+	66.701
1.3963	6	1	2	4+	66.964
1.3899	6	-4	3	3	67.311
1.3861	7	6	2	2	67.522
1.3769	4	1	4	3+	68.034
1.3620	1	-2	4	3	68.884
1.3553	2	1	5	2	69.274
1.3519	2	2	2	4	69.472
1.3507	4	3	1	4+	69.544
1.3460	6	-6	1	3	69.819
1.3392	5	-3	2	4	70.225
1.3371	8	4	3	3+	70.351
1.3261	4	4	5	0	71.027
1.3166	4	8	0	0	71.617
1.3049	2	-5	4	2	72.357
1.2971	6	7	3	0	72.862

Barium Titanium Oxide, $Ba_4Ti_{13}O_{30}$

Synonym
Barium titanate
Tetrabarium 13-titanate

Sample
The sample was prepared from stoichiometric amounts of $BaTiO_3$ and TiO_2. The mixture was heated at 1000°C for one day, then ground and heated further at 1280°C for about 43 hours.

Color
Colorless

Symmetry classifications

Crystal System	Orthorhombic
Space Group	Abma (64)
Pearson Symbol	oC188

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 Å
2θ Standard	Ag
Scanned to	4.0° 2θ
$\sigma(I^{rel})$	±4

Crystallographic constants of this sample
a = 14.059 (2) Å
b = 17.065 (2)
c = 9.8679 (12)

a/b = 0.8238
c/b = 0.5783

V = 2367.48 $Å^3$
Z = 4
Density (calc.) = 4.635 g/cm^3

Figures of merit
F_{30} = 71.0(.0064, 66)
M_{20} = 45.9

Comments
The structure was determined by Tillmanns (#1) and Negas et al. (#2). The cell reported here is pseudo-hexagonal with "a"=~9.858 and "c"=~14.060. The mean temperature of data collection was 24.5°C.

Additional patterns
PDF card 26-762
Rase and Roy (#3) reported as $BaTi_3O_7$

References
#1. Tillmanns, E.
Inorg. Nucl. Chem. Lett.(1971) 7,1169.
#2. Negas, T. et al.
J. Solid State Chem.(1974) 9,297.
#3. Rase, D.E. and Roy, R.
J. Am. Chem. Soc.(1955) 38,102.

d(Å)	I^{rel}	hkl	2θ(°)
8.54	7	0 2 0	10.351
5.429	9	2 1 1+	16.314
4.933	3	0 0 2	17.967
4.651	21	1 3 1+	19.068
4.268	48	0 4 0+	20.794
4.089	8	1 2 2	21.717
4.036	42	2 3 1+	22.004
3.647	4	2 4 0+	24.387
3.516	12	4 0 0	25.309
3.399	21	3 0 2+	26.200
3.251	45	4 1 1+	27.411
3.148	100	1 1 3+	28.332
2.931	31	2 5 1+	30.469
2.861	61	4 3 1+	31.240
2.843	17	0 6 0	31.442
2.791	50	1 3 3	32.047
2.714	13	4 2 2+	32.975
2.6706	33	5 1 1	33.529
2.6568	63	3 5 1+	33.708
2.6377	7	2 6 0+	33.959
2.4638	9	0 6 2	36.438
2.4422	12	5 3 1+	36.771
2.3763	3	4 5 1+	37.829
2.3690	3	0 2 4	37.951
2.3429	11	6 0 0	38.390
2.3343	13	1 7 1+	38.536
2.3282	9	2 0 4	38.642
2.2597	4	6 1 1+	39.861
2.2436	18	2 7 1+	40.159
2.2134	6	4 3 3	40.732
2.1824	61	3 0 4+	41.337
2.1325	3	0 8 0	42.350
2.1205	17	5 1 3+	42.602
2.1155	19	3 2 4+	42.708
2.0532	9	6 4 0+	44.069
2.0181	48	4 6 2+	44.877
2.0011	12	5 3 3	45.279
1.9642	16	4 5 3+	46.180
1.9431	24	3 4 4	46.709
1.9397	27	1 7 3+	46.798
1.8955	6	6 5 1+	47.956
1.8884	5	2 1 5	48.148
1.8603	14	7 0 2+	48.923
1.8540	30	5 0 4+	49.100
1.8248	18	4 4 4	49.938
1.8176	5	7 2 2	50.149
1.8114	10	5 5 3+	50.332
1.8065	10	3 8 2+	50.478
1.8026	13	2 3 5+	50.597
1.7317	5	3 6 4+	52.825
1.7209	7	8 2 0+	53.181
1.7069	4	0 10 0+	53.654
1.7048	5	7 5 1+	53.724
1.7007	6	5 4 4	53.862
1.6600	9	2 5 5	55.295

continued

Barium Titanium Oxide, $Ba_4Ti_{13}O_{30}$ (continued)

d(A)	I^{rel}	hkl	2θ(°)
1.6552	14	8 3 1+	55.469
1.6477	9	4 3 5+	55.743
1.6445	16	0 0 6+	55.863
1.6406	9	7 3 3	56.005
1.6247	3	8 4 0+	56.603
1.6127	5	0 10 2	57.063
1.6071	12	5 7 3+	57.282
1.6041	11	1 2 6	57.397
1.5776	5	6 8 0	58.455
1.5718	5	2 10 2	58.690
1.5572	21	7 6 2+	59.298
1.5535	15	5 6 4+	59.450
1.5365	6	4 5 5+	60.177
1.5321	10	7 2 4+	60.366
1.5256	15	1 4 6+	60.653
1.4996	6	2 4 6+	61.816
1.4975	15	2 11 1	61.912
1.4944	9	8 6 0+	62.056
1.4894	7	9 0 2+	62.287
1.4632	6	7 4 4	63.530
1.4594	5	6 3 5+	63.719
1.4313	18	8 0 4+	65.119
1.4242	23	0 6 6	65.484
1.4111	9	8 7 1+	66.171
1.4061	16	9 4 2+	66.437
1.3991	7	5 10 2+	66.814

Barium Titanium Oxide, $Ba_6Ti_{17}O_{40}$

Synonym
Hexabarium 17-titanate

Sample
The sample was prepared from stoichiometric amounts of $BaTiO_3$ and TiO_2. The mixture was heated at 1000°C for one day, then ground, and heated further at 1280°C for about 43 hours.

Color
Colorless

Symmetry classifications
Crystal System Monoclinic
Space Group A2/a (15)
Pearson Symbol mC252

Data collection and analysis parameters
Radiation $CuK\alpha_1$
Wavelength 1.5405981 A
2θ Standard Ag FP
Scanned to 5.0° 2θ
$\sigma(I^{rel})$ ±3

Crystallographic constants of this sample
a = 18.930 (2) A
b = 17.103 (2)
c = 9.8913 (11)
β = 98.74 (1)°

a/b = 1.1068
c/b = 0.5783

V = 3165.22 A^3
Z = 4
Density (calc.) = 4.781 g/cm^3

Figures of merit
F_{30} = 67.4(.0072, 62)
M_{20} = 23.3

Comments
The structure was determined by Tillmanns and Baur (#1).
The mean temperature of data collection was 24.5°C.

Additional patterns
PDF card 26-321

Reference
#1. Tillmanns, E. and Baur, W.H.
Acta Crystallogr., Sect. B(1970) B26,1645.

d(A)	I^{rel}	hkl	2θ(°)
8.54	8	0 2 0	10.351
7.785	10	1 2 0	11.357
6.315	8	2 2 0	14.012
5.913	5	2 1 1	14.971
4.733	9	3 1 1	18.733
4.674	19	1 3 1+	18.970
4.632	3	-2 0 2	19.144
4.273	3	0 4 0	20.772
4.226	4	2 3 1	21.007
4.168	48	1 4 0	21.301
4.075	2	-2 2 2	21.793
4.028	3	1 2 2	22.049
3.888	5	2 4 0+	22.852
3.749	15	-3 2 2	23.716
3.729	38	3 3 1	23.843
3.688	4	2 2 2	24.111
3.671	3	-4 0 2	24.227
3.604	7	-5 1 1	24.684
3.524	3	3 4 0+	25.253
3.429	3	5 2 0	25.966
3.268	28	5 1 1+	27.263
3.229	31	0 5 1+	27.604
3.201	38	0 1 3	27.851
3.178	56	-2 1 3	28.058
3.149	59	4 0 2	28.321
3.118	31	6 0 0+	28.604
3.096	80	-5 3 1	28.809
3.080	58	1 1 3	28.971
3.061	76	-6 1 1	29.155
3.037	10	-3 1 3	29.386
2.984	67	-3 4 2	29.917
2.957	3	4 2 2+	30.203
2.931	3	6 2 0+	30.472
2.853	100	-1 3 3	31.326
2.831	24	-6 0 2+	31.575
2.811	39	3 5 1+	31.810
2.750	9	3 4 2	32.537
2.730	6	-6 3 1	32.776
2.723	7	-4 5 1	32.866
2.714	7	-3 3 3	32.983
2.688	6	-6 2 2+	33.300
2.652	10	-7 1 1	33.776
2.639	16	5 2 2	33.947
2.597	19	4 5 1	34.515
2.571	4	-5 4 2	34.867
2.551	7	7 2 0	35.150
2.5200	3	6 4 0	35.598
2.5077	4	-5 5 1	35.778
2.4749	3	4 1 3	36.268
2.4638	12	6 0 2+	36.437
2.4577	13	-2 0 4	36.532
2.4280	11	-7 3 1+	36.994
2.3603	3	-6 4 2+	38.095
2.3492	16	-2 5 3	38.282
2.3389	23	8 0 0+	38.458

continued

Barium Titanium Oxide, $Ba_6Ti_{17}O_{40}$ (continued)

d(A)	I^{rel}	hkl			2θ(°)
2.3278	16	5	4	2	38.649
2.3020	6	-6	5	1	39.100
2.2910	13	4	3	3+	39.295
2.2823	42	2	0	4	39.451
2.2778	37	2	7	1+	39.531
2.2662	20	7	4	0+	39.743
2.2508	36	-4	6	2	40.025
2.2314	12	2	5	3+	40.389
2.1891	5	3	7	1+	41.204
2.1465	4	-4	7	1	42.061
2.1400	15	-1	4	4	42.194
2.1132	54	4	6	2	42.756
2.0831	42	-6	0	4+	43.405
2.0777	39	1	4	4	43.523
2.0423	8	4	0	4	44.317
2.0366	15	-5	7	1+	44.447
2.0195	6	4	5	3+	44.844
2.0088	15	-6	6	2+	45.096
1.9887	11	-8	4	2+	45.577
1.9701	6	-9	3	1+	46.032
1.9607	14	-1	8	2+	46.265
1.9552	19	0	7	3	46.405
1.9495	16	-2	7	3+	46.547
1.9442	9	4	8	0	46.681
1.9216	15	-6	7	1	47.264
1.9086	6	-7	2	4	47.606
1.9035	7	5	5	3+	47.742
1.8982	6	-4	1	5	47.882
1.8709	20	10	0	0+	48.626
1.8648	30	9	3	1+	48.797
1.8475	10	2	1	5+	49.283
1.8431	14	4	4	4+	49.410
1.8347	22	-8	0	4	49.650
1.8069	3	-7	7	1+	50.467
1.7959	8	6	0	4	50.798
1.7919	9	-9	3	3	50.919
1.7798	16	3	1	5+	51.291
1.7645	15	-8	6	2	51.767
1.7605	13	-8	5	3	51.896
1.7288	3	-6	7	3	52.919
1.7078	17	3	3	5	53.623
1.7034	15	1	10	0	53.771
1.6818	9	-6	6	4+	54.519
1.6685	5	11	2	0+	54.990
1.6601	6	4	6	4	55.291
1.6477	12	-2	0	6+	55.744
1.6346	9	8	6	2+	56.231
1.6282	7	-7	8	2	56.473

Beryllium Oxide, BeO

Mineral name
Bromellite, syn
Wurtzite Group
Zincite Subgroup

CAS registry no.
1304-56-9

Sample
The sample was obtained from Alfa Products, Thiokol/Ventron Division, Danvers, MA.

Color
Colorless

Symmetry classifications

Crystal System	Hexagonal
Space Group	$P6_3mc$ (186)
Pearson Symbol	$hP4$

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±1

Crystallographic constants of this sample
a = 2.69808 (8) A
c = 4.3785 (2)

c/a = 1.6228

V = 27.60 A^3
Z = 2
Density (calc.) = 3.009 g/cm^3

Figures of merit
F_{18} = 137.0(.0073, 18)
M_{18} = 437.4

Comments
The structure was determined by Zachariasen (#1).
The temperature of data collection was approximately 25.0°C.

Additional patterns
PDF card 4-843, Swanson, H.E. and Tatge, E. (1953). Natl. Bur. Stand. Circ. 539,1, 36.
Zachariasen (#1)
Hanawalt et al. (#2)
Claassen (#3)

References

#1. Zachariasen, W.H.
Z. Phys. Chem. (Leipzig)(1926) 119,201.
#2. Hanawalt, et al.
Ind. Eng. Chem., Anal. Ed.(1938) 10,457.
#3. Claassen, A.
Z. Phys. Chem. (Leipzig)(1926) 124,139.

d(A)	I^{rel}	hkl	2θ(°)
2.3370	85	1 0 0	38.491
2.1888	56	0 0 2	41.210
2.0615	100	1 0 1	43.884
1.5975	19	1 0 2	57.658
1.3493	28	1 1 0	69.625
1.2378	22	1 0 3	76.972
1.1683	4	2 0 0	82.501
1.1486	14	1 1 2	84.232
1.1288	4	2 0 1	86.061
1.0948	1	0 0 4	89.438
1.0309	2	2 0 2	96.704
0.9913	1L	1 0 4	101.989
0.91200	5	2 0 3	115.263
0.88318	2	2 1 0	121.428
0.86569	2	2 1 1	125.699
0.85000	1	1 1 4	129.981
0.81999	5	1 0 5	139.902
0.81901	2	2 1 2	140.280

Bismuth Dysprosium Titanium Oxide, $Bi_{3.6}Dy_{0.4}Ti_3O_{12}$

Sample

The sample was made by combining $Bi_4Ti_3O_{12}$ with TiO_2 and Dy_2O_3. The mixture was heated at 900°C for 18 hours, then at 1050°C for 22 hours.

Color

Grayish greenish yellow

Symmetry classifications

Crystal System	Orthorhombic
Space Group	C***
Pearson Symbol	oC76

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	FP W
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample

a = 5.4256 (5) A
b = 32.783 (2)
c = 5.3923 (6)

a/b = 0.1655
c/b = 0.1645

V = 959.29 A^3
Z = 4
Density (calc.) = 7.984 g/cm^3

Figures of merit

F_{30} = 56.2(.0086, 62)
M_{20} = 37.4

Comments

In 1950, Aurivillius (#1) proposed a face-centered structure for the phase $Bi_4Ti_3O_{12}$. Wolfe and Newnham (#2) reported the existence of comparable solid solution phases in which rare earths substitute for small amounts of the bismuth. Those phases appear to have orthorhombic symmetry, point group mm2, but could possibly be monoclinic. Our data could not be indexed using an F-centered cell and is shown here indexed on a C-centered cell. The mean temperature of data collection was 25.1°C.

References

#1. Aurivillius, B.
Ark. Kemi(1950) 1,499.
#2. Wolfe, R.W. and Newnham, R.E.
J. Electrochem. Soc.(1969) 116,832.

d(A)	I^{rel}	hkl	2θ(°)
16.47	4	0 2 0	5.361
8.20	6	0 4 0	10.781
5.463	16	0 6 0	16.212
4.507	1L	0 4 1	19.683
4.096	12	0 8 0	21.679
3.799	19	1 1 1	23.398
3.610	3	1 3 1	24.640
3.302	6	1 5 1	26.980
3.277	2	0 10 0	27.190
2.962	100	1 7 1	30.145
2.731	8	0 12 0	32.766
2.711	21	2 0 0	33.010
2.695	19	0 0 2	33.220
2.637	1L	1 9 1	33.974
2.574	1	2 4 0	34.828
2.560	1	0 4 2	35.026
2.430	3	2 6 0	36.969
2.417	3	0 6 2	37.162
2.351	7	1 11 1	38.251
2.342	14	0 14 0	38.410
2.262	10	2 8 0	39.818
2.252	12	0 8 2	39.995
2.1054	4	1 13 1	42.923
2.0831	1L	0 10 2	43.404
2.0491	2	0 16 0	44.163
1.9253	3	2 12 0	47.167
1.9194	8	0 12 2	47.321
1.9123	16	2 0 2	47.507
1.8976	9	1 15 1	47.900
1.8616	1L	2 4 2	48.885
1.8215	1	0 18 0	50.035
1.8050	2	2 6 2+	50.525
1.7727	13	2 14 0	51.510
1.7681	16	0 14 2	51.654
1.7441	1L	1 13 2+	52.420
1.7336	3	2 8 2	52.761
1.7220	2	1 17 1	53.146
1.7127	3	3 1 1	53.456
1.7043	2	1 1 3	53.741
1.6593	1L	3 5 1	55.321
1.6512	1	1 5 3+	55.616
1.6347	1L	2 16 0	56.228
1.6307	1L	0 16 2	56.377
1.6102	12	3 7 1	57.159
1.6032	16	1 7 3	57.434
1.5728	4	1 19 1	58.652
1.5687	2	0 20 1	58.817
1.5123	1L	2 18 0	61.241
1.5090	1L	0 18 2	61.390
1.4902	2	0 22 0	62.250
1.4864	3	3 11 1	62.428
1.4813	8	2 14 2+	62.666
1.4454	7	1 21 1+	64.407
1.4181	1L	3 13 1	65.802
1.4131	1L	1 13 3	66.067

continued

d(A)	I^{rel}	hkl	2θ(°)
1.4035	1L	1 19 2	66.575
1.3983	1	2 16 2	66.855
1.3658	1L	0 24 0	68.664
1.3559	1	4 0 0	69.234
1.3486	4	3 15 1	69.664
1.3448	4	1 15 3	69.889
1.3357	1	1 23 1	70.438
1.3192	1L	3 17 0+	71.452
1.3158	1L	4 0 1	71.667
1.3060	1	2 22 0	72.286
1.3043	2	0 22 2	72.396
1.2807	1L	0 8 4	73.951
1.2778	1L	1 17 3	74.145
1.2743	1	1 25 0+	74.381
1.2608	1L	0 26 0	75.315
1.2404	1L	1 25 1	76.779

Bismuth Titanium Oxide, $Bi_4Ti_3O_{12}$

Synonym
Tetrabismuth trititanium dodecaoxide

CAS registry no.
12010-77-4

Sample
The sample was obtained from CERAC, Inc., Milwaukee, WI, and contained about 2% (by volume) of $Bi_{12}TiO_{20}$. The impurity did not interfere with our data measurements.

Spectrographic analysis (wt.%, CERAC, Inc.)
0.001 Ca, Fe, Mg
0.005 Al, Cu, Sn
0.008 Si

Color
Yellowish gray

Symmetry classifications

Crystal System	Orthorhombic
Space Group	C***
Pearson Symbol	oC76

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	FP W
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±1

Crystallographic constants of this sample
a = 5.4489 (5) A
b = 32.815 (2)
c = 5.4100 (5)

a/b = 0.1660
c/b = 0.1649

V = 967.34 A^3
Z = 4
Density (calc.) = 8.045 g/cm^3

Figures of merit
F_{30} = 61.2(.0078, 63)
M_{20} = 52.7

Comments
Aurivillius (#1) proposed the space group Fmmm. Our data is inconsistent with Fmmm and is presented here using C***. By a detailed study of the optical properties of a single crystal, Cummins and Cross (#2) concluded that the true symmetry is monoclinic, point group m; however, we found no problem when indexing the powder data with the orthorhombic cell given here.
A phase change takes place at 676°C (#2).
The mean temperature of data collection was 23.4°C.

Additional patterns
PDF card 12-213

References
#1. Aurivillius, B.
Ark. Kemi(1950) 1,499.
#2. Cummins, S.E. and Cross, L.E.
J. Appl. Phys.(1968) 39,2268.

d(Å)	I^{rel}	hkl	2θ(°)
16.48	1L	0 2 0	5.359
8.21	4	0 4 0	10.773
5.469	14	0 6 0	16.195
4.519	1L	0 4 1	19.627
4.101	8	0 8 0	21.651
3.813	20	1 1 1	23.307
3.623	2	1 3 1	24.553
3.311	5	1 5 1	26.903
3.281	2	0 10 0	27.156
2.971	100	1 7 1	30.058
2.734	14	0 12 0	32.725
2.725	24	2 0 0	32.843
2.705	19	0 0 2	33.095
2.645	1L	1 9 1	33.867
2.585	1	2 4 0	34.668
2.570	1L	0 4 2	34.885
2.4383	4	2 6 0+	36.832
2.4247	4	0 6 2	37.046
2.3566	6	1 11 1	38.158
2.3436	13	0 14 0	38.378
2.2697	12	2 8 0	39.679
2.2581	12	0 8 2	39.891
2.1090	4	1 13 1	42.846
2.0504	2	0 16 0	44.132
1.9307	6	2 12 0	47.028
1.9193	17	2 0 2	47.325
1.9007	9	1 15 1	47.816
1.8815	1L	1 11 2	48.334
1.8684	1	2 4 2	48.696
1.8229	2	0 18 0	49.993
1.8112	2	2 6 2	50.339
1.7771	12	2 14 0	51.375
1.7716	15	0 14 2	51.546
1.7479	2	1 13 2	52.298
1.7386	4	2 8 2	52.598
1.7246	3	1 17 1	53.058
1.7197	4	3 1 1	53.222
1.7094	2	1 1 3	53.569
1.7012	1	3 3 1	53.848
1.6647	1L	3 5 1	55.125
1.6564	1	1 5 3+	55.425
1.6504	1L	0 8 3	55.647
1.6404	1	0 20 0	56.015
1.6161	14	3 7 1	56.933
1.6080	15	1 7 3	57.245

continued

d(Å)	I^{rel}	hkl	2θ(°)
1.5749	4	1 19 1	58.564
1.5709	4	2 12 2	58.729
1.5150	1	2 18 0	61.119
1.5118	1L	0 18 2	61.265
1.4914	2	3 11 1+	62.196
1.4849	8	1 11 3+	62.500
1.4474	6	1 21 1	64.307
1.4228	1	3 13 1	65.557
1.4168	1	1 13 3	65.871
1.4023	1	0 20 2	66.637
1.3671	1	2 10 3+	68.590
1.3619	1	4 0 0	68.887
1.3530	5	3 15 1+	69.408
1.3484	4	1 15 3+	69.679
1.3374	1L	1 23 1	70.333
1.3218	1	4 6 0+	71.292
1.3125	1L	0 6 4	71.871
1.3084	2	2 22 0	72.136
1.3065	2	0 22 2	72.255
1.2929	1L	4 8 0	73.139
1.2848	1L	3 17 1+	73.673
1.2788	1L	3 1 3	74.082
1.2619	1L	0 26 0	75.239
1.2474	1L	2 20 2	76.269
1.2421	1L	1 25 1	76.658
1.2347	3	3 7 3+	77.199
1.2195	2	3 19 1+	78.344
1.2159	3	1 19 3	78.621
1.2115	2	2 0 4	78.959
1.1877	1L	4 6 2	80.865
1.1845	1	3 21 0	81.129
1.1828	1	2 6 4	81.270
1.1777	3	4 14 0+	81.699
1.1717	3	0 28 0+	82.204
1.1618	1	2 8 4	83.058

Boron Carbide, B_4C

Synonym
Carbon tetraboride

CAS registry no.
12069-32-8

Sample
The compound was obtained from Aesar Division of Johnson Matthey, Inc., Seabrook, NH.

Color
Olive black

Symmetry classifications

Crystal System	Rhombohedral
Space Group	$R\bar{3}m$ (166)
Pearson Symbol	hR15

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±3

Crystallographic constants of this sample
(Hexagonal axes)
a = 5.6003 (5) A
c = 12.086 (2)

c/a = 2.1581

V = 328.27 A^3
Z = 9
Density (calc.) = 2.515 g/cm^3

Figures of merit
F_{25} = 57.6(.0128, 34)
M_{20} = 84.6

Comments
The structure was qualitatively determined by Clark and Hoard (#1).
The mean temperature of data collection was 23.5°C.

Additional patterns
PDF card 6-0555

Reference
#1. Clark, H.K. and Hoard, J.L.
J. Am. Chem. Soc.(1943) 65,2115.

d(A)	I^{rel}	hkl	2θ(°)
4.499	14	1 0 1	19.715
4.033	21	0 0 3	22.022
3.783	49	0 1 2	23.499
2.803	11	1 1 0	31.900
2.565	64	1 0 4	34.957
2.377	100	0 2 1	37.819
2.300	4	1 1 3	39.133
1.8906	1L	0 2 4	48.087
1.8127	4	2 1 1	50.293
1.7120	11	2 0 5	53.480
1.6261	2	1 0 7	56.551
1.5674	1L	2 1 4	58.872
1.5004	9	3 0 3	61.782
1.4605	13	1 2 5	63.663
1.4423	10	0 1 8	64.563
1.3995	12	2 2 0	66.790
1.3369	8	1 3 1	70.363
1.3228	7	2 2 3	71.231
1.3128	8	3 1 2	71.854
1.2820	2	2 0 8	73.863
1.2605	3	3 0 6	75.338
1.2571	6	2 1 7	75.578
1.2112	1L	1 1 9	78.987
1.2065	1	4 0 1	79.351
1.1887	4	0 4 2	80.782

Boron Silicide, B_4Si

Synonym
Silicon tetraboride

CAS registry no.
12007-81-7

Sample
The sample was obtained from CERAC, Inc., Milwaukee, WI. It contains a small amount of other B-Si phases.

Spectorgraphic analysis (wt.%, CERAC, Inc.)
0.1-1.0 Fe
0.1 Cr
0.01 Co, Mo
0.005 Mg, Ni, Sn
0.001 Al, Ca, Cu, Mn, Ti

Color
Black

Symmetry classifications

Crystal System	Rhombohedral
Space Group	$R\bar{3}m$ (166)
Pearson Symbol	hR15

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±1

Crystallographic constants of this sample
(Hexagonal axes)
a = 6.3367 (4) A
c = 12.7447 (16)

c/a = 2.0113

V = 443.19 A^3
Z = 9
Density (calc.) = 2.405 g/cm^3

Figures of merit
F_{30} = 90.4(.0079, 42)
M_{20} = 124.8

Comments
Isostructural with C_4Si (#1).
B_4C has a wide range of composition (#2).
The mean temperature of data collection was 23.0°C.

Additional patterns
PDF card 13-210
Matkovich (#1)

References

#1. Matkovich, V.I.
Acta Crystallogr.(1960) 13,679.
#2. Rizzo, H.F. and Bidwell, L.R.
J. Am. Ceram. Soc.(1960) 43,550.

d(A)	I^{rel}	hkl	2θ(°)
5.039	4	1 0 1	17.585
4.158	30	0 1 2	21.353
3.167	22	1 1 0	28.150
2.754	64	1 0 4	32.488
2.681	100	0 2 1	33.391
2.520	6	2 0 2	35.596
2.3116	6	0 1 5	38.930
2.1242	3	0 0 6	42.524
2.0792	3	0 2 4	43.491
2.0469	14	2 1 1	44.212
1.9724	1	1 2 2	45.976
1.7643	12	1 1 6	51.774
1.7384	3	2 1 4	52.606
1.7282	4	1 0 7	52.940
1.6798	8	3 0 3	54.589
1.6087	26	1 2 5	57.218
1.5843	12	2 2 0	58.185
1.5302	4	0 1 8	60.452
1.5178	9	0 2 7	60.995
1.5111	15	1 3 1	61.295
1.4844	11	2 2 3	62.522
1.4807	12	3 1 2	62.695
1.3858	9	3 0 6	67.539
1.3735	3	1 3 4	68.228
1.3412	1	0 4 2	70.105
1.3072	3	3 1 5	72.211
1.2929	1	1 1 9	73.138
1.2695	1	2 2 6	74.710
1.2351	1	2 3 2	77.169
1.2080	1	0 4 5	79.233
1.1978	1	4 1 0	80.046
1.1706	1	3 2 4	82.298
1.1679	1	1 3 7	82.537

Boron Silicide, B_6Si

Synonym
Silicon hexaboride

CAS registry no.
12008-29-6

Sample
The sample was obtained from CERAC, Inc., Milwaukee, WI. It contained a small amount of silicon. Owing to the poor diffraction characteristics of the sample, the intensities were run on a flat pressed holder and thus may show orientation.

Color
Black

Symmetry classifications

Crystal System	Orthorhombic
Space Group	Pnnm (58)
Pearson Symbol	oP280

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	W FP
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±6

Crystallographic constants of this sample
a = 14.470 (2) A
b = 18.350 (3)
c = 9.946 (2)

a/b = 0.7886
c/b = 0.5420

V = 2640.91 A^3
Z = 40
Density (calc.) = 2.338 g/cm^3

Figures of merit
F_{30} = 41.0(.0099, 74)
M_{20} = 22.4

Comments
The structure was done by Adamsky (#1).
A cubic form was reported by Zhuravlev (#2).
The mean temperature of data collection was 23.6°C.

Additional patterns
PDF card 11-292
PDF card 14-92

References
#1. Adamsky, R.F.
Acta Crystallogr.(1958) 11,744.
#2. Zhuravlev, N.N.
Kristallografiya(1956) 1,66.

d(A)	I^{rel}	hkl	2θ(°)
11.41	9	1 1 0	7.745
7.74	5	1 2 0	11.422
7.51	6	1 1 1	11.782
5.683	8	2 2 0	15.579
5.573	7	2 1 1	15.889
5.214	8	0 3 1	16.991
4.975	75	0 0 2	17.813
4.676	38	2 3 0+	18.965
4.589	2	0 4 0	19.325
4.374	78	1 4 0+	20.285
4.227	84	2 3 1+	20.999
4.186	75	1 2 2	21.208
4.098	65	2 0 2	21.667
4.006	33	1 4 1+	22.175
3.927	13	3 2 1	22.626
3.875	31	2 4 0	22.933
3.742	27	2 2 2	23.757
3.552	13	4 1 0	25.049
3.443	32	0 5 1	25.854
3.405	52	2 3 2+	26.151
3.366	54	4 2 0	26.461
3.342	58	4 1 1	26.652
3.275	43	2 5 0	27.204
3.240	23	3 2 2	27.503
3.188	52	4 2 1	27.969
3.058	24	0 6 0+	29.175
2.972	38	4 3 1+	30.048
2.923	40	4 0 2+	30.555
2.889	47	4 1 2	30.926
2.862	92	2 2 3+	31.230
2.817	52	2 6 0	31.738
2.803	64	3 5 1	31.905
2.777	61	5 0 1	32.207
2.763	71	3 4 2	32.381
2.731	61	4 4 1+	32.767
2.703	100	3 1 3+	33.121
2.659	41	5 2 1	33.680
2.640	64	4 3 2+	33.933
2.619	45	3 2 3	34.211
2.606	44	0 6 2	34.391
2.576	30	4 5 0	34.801
2.563	26	1 6 2	34.981
2.534	27	0 7 1	35.391
2.495	27	3 3 3+	35.970
2.466	19	4 4 2+	36.403
2.448	11	5 4 0	36.683
2.423	30	4 1 3	37.069
2.393	11	2 7 1+	37.554
2.368	33	1 2 4	37.962
2.362	25	4 2 3	38.074
2.351	28	2 0 4	38.244
2.336	6	4 6 0	38.514
2.295	12	0 8 0	39.225
2.288	11	4 5 2	39.355
2.274	25	4 6 1+	39.599

continued

d(A)	I^{rel}	hkl	2θ(°)
2.215	5	5 5 1	40.696
2.189	18	6 3 1	41.216
2.1809	14	5 0 3	41.366
2.1472	14	2 6 3+	42.046
2.0917	8	2 4 4	43.217
2.0667	12	5 5 2	43.767
2.0485	20	4 0 4	44.177
2.0362	20	4 1 4+	44.458
2.0168	20	7 2 0	44.908
2.0113	7	7 1 1	45.038
1.9903	9	3 4 4	45.538
1.9788	13	1 9 1+	45.818
1.9253	14	2 9 1	47.169
1.9218	22	7 3 1	47.259
1.9066	14	5 7 1+	47.659
1.8579	24	6 3 3	48.989
1.8255	17	2 9 2+	49.919
1.7752	18	5 6 3+	51.434
1.7709	15	8 1 1	51.569
1.7572	7	3 9 2+	51.999
1.7475	8	6 7 1+	52.309
1.7355	8	4 1 5+	52.699
1.7227	48	7 2 3+	53.120
1.6892	25	2 9 3+	54.259
1.6864	19	7 3 3+	54.358
1.6593	27	8 4 1	55.322
1.6382	56	7 4 3+	56.094
1.6332	50	5 1 5	56.283
1.6226	28	8 5 0+	56.685

Cadmium Silicate, $CdSiO_3$

Synonym
Cadmium metasilicate

CAS registry no.
13477-19-5

Sample
The sample was made by heating a 1:1 molar mixture of cadmium oxalate and SiO_2 up to 900°C for 3 days followed by heating up to 1175°C for about 6 hours.

Color
Colorless

Symmetry classifications

Crystal System	Monoclinic
Space Group	$P2_1/a$ (14)
Pearson Symbol	mP30
Structure Type	Similar to pseudo-wollastonite $CaSiO_3$

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	FP Ag
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±1

Crystallographic constants of this sample
a = 15.095 (3) Å
b = 3.630 (5)
c = 6.953 (1)
β = 94.799 (14)°

a/b = 4.1584
c/b = 1.9154

V = 379.65 $Å^3$
Z = 6
Density (calc.) = 4.947 g/cm^3

Figures of merit
F_{30} = 84.9(.0065, 54)
M_{20} = 57.9

Comments
The cell was obtained from the Visser program and is similar to one reported by Glasser and Glasser (#1) with bx2.
The mean temperature of data collection was 23.9°C.

Additional patterns
PDF card 16-299

Reference
#1. Glasser, L.S.D. and Glasser, F.P. Inorg. Chem.(1964) 3,1228.

d(A)	I^{rel}	hkl	2θ(°)
7.520	3	2 0 0	11.759
6.935	7	0 0 1	12.754
5.323	3	-2 0 1	16.641
4.898	39	2 0 1	18.097
3.759	8	4 0 0	23.651
3.464	18	0 0 2	25.699
3.426	17	-4 0 1	25.986
3.252	23	-2 0 2	27.408
3.170	15	-1 1 1	28.123
3.119	2	1 1 1	28.600
3.051	26	2 0 2	29.251
2.940	100	3 1 0	30.381
2.756	13	-3 1 1	32.462
2.6596	17	3 1 1+	33.671
2.6123	1L	4 1 0	34.300
2.5063	26	0 1 2+	35.799
2.4951	24	-1 1 2	35.964
2.4478	35	4 0 2+	36.684
2.4220	3	-2 1 2+	37.090
2.3173	10	5 1 0	38.830
2.3093	10	0 0 3	38.970
2.2981	4	-3 1 2	39.168
2.2620	21	-2 0 3	39.820
2.2407	3	-5 1 1	40.215
2.1899	3	3 1 2	41.189
2.1551	32	5 1 1	41.885
2.1163	2	-6 0 2	42.690
1.9857	3	-5 1 2	45.650
1.9550	2	6 0 2	46.410
1.9150	9	1 1 3	47.437
1.8986	3	4 0 3	47.873
1.8788	2	8 0 0	48.408
1.8699	4	5 1 2	48.653
1.8497	4	7 1 0	49.220
1.8191	16	-7 1 1	50.106
1.8147	17	0 2 0	50.234
1.7772	10	8 0 1	51.370
1.7562	1	0 2 1	52.033
1.7314	11	0 0 4	52.833
1.7014	7	2 2 1	53.840
1.6910	16	-5 1 3	54.197
1.6818	14	4 1 3	54.520
1.6322	2	6 0 3	56.320
1.6261	1L	-4 0 4	56.552
1.6072	3	0 2 2	57.276
1.6042	2	-4 2 1	57.395
1.5846	15	7 1 2	58.170
1.5604	3	2 2 2	59.162
1.5252	7	-3 1 4+	60.671

Cadmium Titanium Phosphate, $CdTi_4(PO_4)_6$

Sample

The sample was prepared from $CdCO_3$, $(NH_4)_2HPO_4$, and TiO_2 in stoichiometric ratios of 1:6:4. The mixture was ground and heated slowly to 500°C, then reground and heated at 1250°C for 15 hours.

Color

Colorless

Symmetry classifications

Crystal System	Rhombohedral
Space Group	R**
Pearson Symbol	hR35

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	Ag FP
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±3

Crystallographic constants of this sample
(Hexagonal axes)

a = 8.4511 (3) A
c = 21.5457 (13)

c/a = 2.5495

V = 1332.65 A^3
Z = 3
Density (calc.) = 3.266 g/cm^3

Figures of merit

F_{30} = 149.9(.0059, 34)
M_{20} = 108.2

Comments

Apparently rhombohedral, from analogy with the powder pattern of $SrZr_4(PO_4)_6$.
The structure appears to be very similar to that of $NaZr_2(PO_4)_3$.
The mean temperature of data collection was 25.5°C.

d(A)	I^{rel}	hkl	2θ(°)
7.197	16	0 0 3	12.289
6.933	29	1 0 1	12.758
4.339	8	1 0 4	20.453
4.226	53	1 1 0	21.003
3.713	16	0 1 5	23.944
3.641	100	1 1 3	24.426
3.608	8	0 2 1	24.658
3.465	13	2 0 2	25.693
3.027	10	0 2 4	29.490
2.838	4	1 0 7	31.500
2.7895	6	2 0 5	32.060
2.7448	25	2 1 1	32.597
2.7360	67	1 1 6	32.704
2.6793	8	1 2 2	33.417
2.5279	3	0 1 8	35.483
2.4600	1	2 1 4	36.496
2.4397	20	3 0 0	36.810
2.3565	1	0 2 7	38.160
2.3280	8	1 2 5	38.645
2.3099	6	3 0 3	38.959
2.1689	5	2 0 8	41.605
2.1119	1	2 2 0	42.784
2.0828	7	1 1 9	43.411
2.0669	2	1 0 10	43.762
2.0573	7	2 1 7	43.977
2.0266	7	2 2 3	44.680
2.0214	8	1 3 1	44.801
2.0176	6	3 0 6	44.890
1.9299	18	1 2 8	47.049
1.8994	1	1 3 4	47.850
1.8919	2	0 1 11	48.052
1.8362	4	3 1 5	49.607
1.8212	18	2 2 6	50.044
1.8040	1	0 4 2	50.553
1.7952	4	0 0 12	50.818
1.7323	1	4 0 4	52.803
1.7271	2	2 0 11	52.975
1.7081	1L	3 0 9	53.610
1.7004	3	2 1 10	53.873
1.6949	6	1 3 7	54.063
1.6838	1	0 4 5	54.448
1.6738	1	3 2 1	54.800
1.6590	2	2 3 2	55.332
1.6208	9	3 1 8	56.753
1.6165	6	1 0 13	56.917
1.6030	3	3 2 4	57.442
1.5970	13	4 1 0	57.675
1.5839	2	2 2 9	58.200
1.5727	1	4 0 7	58.656
1.5643	3	2 3 5	59.000
1.5596	4	4 1 3	59.197
1.5132	5	0 4 8	61.203
1.5096	4	0 2 13	61.362
1.5057	3	0 1 14	61.540
1.4772	3	1 3 10	62.859
1.4741	3	3 2 7	63.009
1.4592	8	4 1 6	63.726
1.4461	2	3 0 12	64.373
1.4249	2	2 3 8	65.450
1.4221	2	2 1 13	65.593
1.4185	6	2 0 14	65.781
1.4094	6	3 1 11	66.261
1.3951	1L	4 0 10	67.031
1.3859	1	5 0 5	67.531
1.3823	2	3 3 3	67.735
1.3602	2	1 1 15	68.986
1.3449	4	1 2 14	69.886
1.3370	1L	0 4 11	70.362
1.3286	1	4 1 9	70.870
1.3170	1	4 2 5	71.588

continued

Cadmium Titanium Phosphate, $CdTi_4(PO_4)_6$ (continued)

d(A)	I^{rel}	hkl	2θ(°)
1.3120	4	5 1 1	71.908
1.3051	1	1 5 2	72.349
1.2837	2	1 3 13	73.748
1.2770	2	5 1 4	74.203
1.2616	1	2 4 7	75.263
1.2573	2	1 5 5	75.563
1.2302	1	4 2 8	77.536
1.2264	3	3 1 14	77.823
1.2201	3	6 0 0	78.299
1.2088	2	5 1 7	79.172

Calcium Aluminum Silicate, $Ca_2Al_2SiO_7$

Mineral name
Gehlenite, syn
Melilite Group

Sample
The sample was prepared by blending $CaCO_3$, Al_2O_3, and SiO_2 in the appropriate molar ratio. After an initial calcine at a low temperature to remove CO_2, the sample was heated for an extended period in the 1200-1400°C range with periodic grinding.

Color
Colorless

Symmetry classifications
Crystal System Tetragonal
Space Group $P\bar{4}2_1m$ (113)
Pearson Symbol $tP24$
Structure Type $Ca_2MgSi_2O_7$, akermanite

Data collection and analysis parameters
Radiation $CuK\alpha_1$
Wavelength 1.5405981 A
2θ Standards W FP
Scanned to 5.0° 2θ
$\sigma(I^{rel})$ ±3

Crystallographic constants of this sample
a = 7.6858 (2) A
c = 5.0683 (2)

c/a = 0.6594

V = 299.39 A^3
Z = 2
Density (calc.) = 3.042 g/cm^3

Figures of merit
F_{30} = 248.2(.0038, 32)
M_{20} = 215.2

Comments
The structure was determined by Raaz (#1) and by Louisnathan (#2).
The mean temperature of data collection was 24.3°C.

Additional patterns
PDF card 20-199
PDF card 25-123
Negro and Regourd (#3)

References

#1. Raaz, F.
Sitzungsber. Akad. Wiss. Wien, Math.-Naturwiss. Kl., Abt. 1(1930) 139,645.
#2. Louisnathan, S.J.
Can. Mineral.(1971) 10,822.
#3. Negro, M.A. and Regourd, M.
Silic. Ind.(1968) 33,137.

d(A)	I^{rel}	hkl	2θ(°)
5.433	4	1 1 0	16.302
5.069	3	0 0 1	17.483
4.231	2	1 0 1	20.979
3.842	1	2 0 0	23.132
3.707	15	1 1 1	23.987
3.4365	2	2 1 0	25.906
3.0629	21	2 0 1	29.132
2.8446	100	2 1 1	31.423
2.7175	5	2 2 0	32.933
2.5339	4	0 0 2	35.396
2.4306	17	3 1 0	36.954
2.4070	11	1 0 2	37.329
2.3944	12	2 2 1	37.533
2.2968	7	1 1 2	39.191
2.2869	11	3 0 1	39.368
2.1917	2	3 1 1	41.153
2.1155	1	2 0 2	42.708
2.0398	9	2 1 2	44.374
1.9651	2	3 2 1	46.156
1.9213	8	4 0 0	47.271
1.8641	4	4 1 0	48.816
1.8535	2	2 2 2	49.114
1.8115	8	3 3 0	50.329
1.7964	1L	4 0 1	50.783
1.7542	25	3 1 2	52.095
1.7495	17	4 1 1	52.247
1.7186	6	4 2 0	53.258
1.7059	3	3 3 1	53.686
1.6891	1L	0 0 3	54.264
1.6498	1L	1 0 3	55.666
1.6314	2	3 2 2	56.352
1.6271	2	4 2 1	56.513
1.6129	2	1 1 3	57.054
1.5463	1L	2 0 3	59.758
1.5309	1L	4 0 2	60.418
1.5162	9	2 1 3	61.067
1.5074	1L	5 1 0	61.462
1.5013	1L	4 1 2	61.739
1.4735	2	3 3 2	63.035
1.4710	2	4 3 1	63.155
1.4448	2	5 1 1	64.439
1.4349	3	2 2 3	64.936
1.4276	1L	5 2 0	65.308
1.4224	2	4 2 2	65.576
1.4101	1	3 0 3	66.224
1.3874	2	3 1 3	67.450
1.3738	9	5 2 1	68.209
1.3586	3	4 4 0	69.079
1.3239	1	3 2 3	71.163
1.3179	1L	5 3 0	71.532
1.3143	2	4 3 2	71.757
1.3123	1	4 4 1	71.889
1.2810	3	6 0 0	73.931
1.2670	2	0 0 4	74.887
1.2636	2	6 1 0	75.124

continued

Calcium Aluminum Silicate, $Ca_2Al_2SiO_7$ (continued)

d(A)	I^{rel}	hkl			2θ(°)
1.2517	5	4	1	3	75.962
1.2435	1	5	2	2	76.555
1.2355	1L	3	3	3	77.138
1.2260	1	6	1	1	77.850
1.20459	1L	4	2	3	79.505
1.20023	1L	5	4	0	79.851
1.19748	1L	4	4	2	80.072
1.18916	1L	2	1	4	80.747
1.18178	1	6	2	1	81.357
1.16801	2	5	4	1	82.523
1.14857	1L	2	2	4	84.236
1.14581	2	6	3	0	84.486
1.14325	1	6	0	2	84.719
1.13581	1	3	0	4	85.405
1.13063	1L	6	1	2	85.891
1.12472	3	5	1	3	86.452
1.09596	1L	6	2	2	89.313
1.09032	2	5	2	3	89.900

Calcium Fluoride, CaF_2

Mineral name
Fluorite, syn
Fluorite Group
Fluorite Subgroup

CAS registry no.
7789-75-5

Sample
The sample was obtained from the U.S. Geological Survey.

Color
Colorless

Symmetry classifications

Crystal System	Cubic
Space Group	Fm3m (225)
Pearson Symbol	cF12
Structure Type	CaF_2

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	W
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample
a = 5.46305 (8) A

V = 163.04 A^3
Z = 4
Density (calc.) = 3.181 g/cm^3

Figures of merit
F_{16} = 213.5(.0047, 16)
M_{16} = 796.2

Comments
The structure was determined by Bragg (#1).
These data were recollected to add weak peaks missing in the earlier pattern.
The mean temperature of data collection was 24.5°C.

Additional patterns
PDF card 4-864, Swanson, H.E. and Tatge,E (1953).
Natl. Bur. Stand. Circ. 539,1,69.
Hanawalt et al. (#2)

References
#1. Bragg, W.L.
Proc. R. Soc. London, Ser. A(1914) 89,468.
#2. Hanawalt, J.D. et al.
Ind. Eng. Chem., Anal. Ed.(1938) 10,457.

d(A)	I^{rel}	hkl	2θ(°)
3.155	92	1 1 1	28.267
2.7314	1L	2 0 0	32.761
1.9316	100	2 2 0	47.005
1.6471	33	3 1 1	55.765
1.5771	1	2 2 2	58.476
1.3656	10	4 0 0	68.674
1.2533	9	3 3 1	75.850
1.2216	1	4 2 0	78.184
1.11523	17	4 2 2	87.372
1.05140	7	3 3 3	94.217
0.96576	4	4 4 0	105.804
0.92340	6	5 3 1	113.064
0.91046	1	6 0 0	115.570
0.86375	8	6 2 0	126.202
0.83314	3	5 3 3	135.208
0.82358	2	6 2 2	138.555

Calcium Germanium Phosphate, $CaGe_4(PO_4)_6$

Synonym
Calcium germanium orthophosphate

Sample
The sample was made by heating a 1:4:6 molar mixture of $CaCO_3$, GeO_2, and $(NH_4)H_2PO_4$ up to 500°C. It was then reground and heated at 1000°C overnight.

Color
Colorless

Symmetry classifications

Crystal System	Rhombohedral
Space Group	R**
Pearson Symbol	hR35
Structure Type	$NaZr_2(PO_4)_3$

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±3

Crystallographic constants of this sample
(Hexagonal axes)
a = 8.0125 (5) A
c = 21.710 (2)

c/a = 2.7095

V = 1207.05 A^3
Z = 3
Density (calc.) = 3.715 g/cm^3

Figures of merit
F_{30} = 99.3(.0082, 37)
M_{20} = 77.3

Comments
The structure of $NaZr_2(PO_4)_3$ has been determined by Hagman and Kierkegaard (#1) and confirmed by Hong (#2).
The mean temperature of data collection was 24.4°C.

References

#1. Hagman, L-O. and Kierkegaard, P.
Acta Chem. Scand.(1968) 22,1822.
#2. Hong, H. Y-P.
Mater. Res. Bull.(1976) 11,173.

d(A)	I^{rel}	hkl	2θ(°)
7.244	4	0 0 3	12.208
6.606	6	1 0 1	13.392
5.846	30	0 1 2	15.143
4.276	60	1 0 4	20.758
4.006	64	1 1 0	22.170
3.684	1	0 1 5	24.137
3.619	4	0 0 6	24.580
3.506	94	1 1 3	25.385
3.427	11	0 2 1	25.977
2.922	61	0 2 4	30.567
2.832	3	1 0 7	31.561
2.685	100	1 1 6	33.340
2.604	16	2 1 1	34.408
2.550	1	1 2 2	35.159
2.528	4	0 1 8	35.482
2.413	1L	0 0 9	37.229
2.3609	15	2 1 4	38.085
2.3124	30	0 2 7+	38.916
2.2443	1	1 2 5	40.146
2.2030	11	3 0 3	40.932
2.1369	5	2 0 8	42.259
2.0666	7	1 1 9	43.769
2.0026	16	2 1 7+	45.245
1.9482	13	3 0 6	46.581
1.9302	2	2 2 3	47.041
1.8944	4	3 1 2	47.984
1.8856	16	1 2 8	48.224
1.8405	12	0 2 10	49.482
1.8143	13	1 3 4	50.248
1.8092	9	0 0 12	50.398
1.7524	27	2 2 6	52.154
1.7297	1L	4 0 1	52.890
1.7132	5	0 4 2	53.440
1.6722	21	2 1 10	54.858
1.6346	4	1 3 7	56.230
1.5880	1	3 2 1	58.033
1.5701	12	3 1 8	58.760
1.5411	2	2 2 9	59.978
1.5279	10	3 2 4	60.553
1.5142	20	4 1 0+	61.155
1.4947	2	2 3 5	62.041
1.4821	2	4 1 3	62.627
1.4618	4	0 4 8	63.599
1.4403	16	1 3 10	64.662
1.4250	3	3 0 12	65.446
1.4160	11	2 0 14+	65.912
1.3968	14	4 1 6	66.935
1.3849	1	0 5 1	67.588
1.3778	1	3 1 11	67.982
1.3728	1	2 3 8	68.268
1.3612	4	1 1 15	68.929
1.3552	6	4 0 10	69.276
1.3446	3	0 5 4	69.905
1.3355	10	3 3 0	70.451

Calcium Titanium Phosphate, $CaTi_4(PO_4)_6$

Synonym
Calcium titanium orthophosphate

Sample
The sample was prepared by heating $Ca_3(PO_4)_2$, $(NH_4)_2HPO_4$, and TiO_2 (anatase) up to 500°C. It was then reground and heated to 1200°C for 3 days.

Color
Colorless

Symmetry classifications

Crystal System	Rhombohedral
Space Group	R**
Pearson Symbol	hR35

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	4.0° 2θ
$\sigma(I^{rel})$	±1

Crystallographic constants of this sample
(Hexagonal axes)
a = 8.3613 (5) A
c = 21.997 (2)

c/a = 2.6308

V = 1331.81 A^3
Z = 3
Density (calc.) = 2.998 g/cm^3

Figures of merit
F_{30} = 97.0(.0081, 38)
M_{20} = 69.4

Comments
Rhombohedral, R** by analogy with other similar titanium phosphates. The structure is similar to $NaZr_2(PO_4)_3$.
The temperature of data collection was approximately 25.0°C.

d(A)	I^{rel}	hkl	2θ(°)
7.332	4	0 0 3	12.061
6.884	6	1 0 1	12.850
6.051	15	0 1 2	14.627
4.382	22	1 0 4	20.250
4.183	28	1 1 0	21.221
3.762	4	0 1 5	23.630
3.634	100	1 1 3	24.479
3.575	2	0 2 1	24.883
3.441	4	2 0 2	25.873
3.025	28	0 2 4	29.510
2.881	1	1 0 7	31.014
2.796	3	2 0 5	31.989
2.757	53	1 1 6	32.446
2.717	16	2 1 1	32.941
2.657	2	1 2 2	33.706
2.451	4	2 1 4	36.638
2.414	13	3 0 0	37.210
2.3239	2	1 2 5	38.716
2.2929	6	3 0 3	39.260
2.1896	2	2 0 8	41.194
2.1102	6	1 1 9	42.820
2.0638	5	2 1 7	43.831
2.0160	5	3 0 6	44.927
2.0105	5	2 2 3	45.057
1.9749	1	3 1 2	45.915
1.9395	12	1 2 8	46.803
1.8865	3	1 3 4	48.199
1.8801	3	0 2 10	48.373
1.8327	3	0 0 12	49.708
1.8270	3	3 1 5	49.874
1.8155	16	2 2 6	50.210
1.8036	7	4 0 1	50.565
1.7862	2	0 4 2	51.095
1.7143	8	2 1 10	53.403
1.6922	5	1 3 7	54.157
1.6555	1	3 2 1	55.458
1.6215	7	3 1 8	56.724
1.5899	6	3 2 4	57.957
1.5799	10	4 1 0	58.362
1.5545	2	2 3 5	59.409
1.5447	2	4 1 3	59.825
1.5355	2	0 1 14	60.221
1.5330	2	0 2 13	60.328
1.5118	3	0 4 8	61.263
1.4828	7	1 3 10	62.597
1.4683	2	3 2 7	63.286
1.4597	5	3 0 12	63.703
1.4506	4	4 1 6	64.147
1.4414	3	2 0 14	64.607
1.4215	1	2 3 8	65.627
1.4169	2	3 1 11	65.866
1.3980	4	4 0 10	66.871
1.3940	4	3 3 0	67.088
1.3844	3	1 1 15	67.619
1.3690	2	3 3 3	68.481
1.3629	5	1 2 14	68.829
1.3578	1	4 2 2	69.124
1.3274	2	4 1 9	70.942
1.3030	1	3 3 6	72.478
1.2983	2	5 1 1	72.787
1.2776	1	2 3 11	74.156
1.2654	5	5 1 4	74.995

Calcium Zinc Silicate, $Ca_2ZnSi_2O_7$

Mineral name
Hardystonite, syn
Melilite Group

Sample
The sample prepared from a 2:1:2 molar mixture of $CaCO_3$, ZnO, and SiO_2 was heated and ground periodically at successively higher temperatures in the range 1150°C to 1325°C.

Color
Colorless

Symmetry classifications

Crystal System	Tetragonal
Space Group	$P\bar{4}2_1m$ (113)
Pearson Symbol	tP24

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 Å
2θ Standards	FP Si
Scanned to	4.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample
a = 7.8250 (3) Å
c = 5.0153 (3)

c/a = 0.6409

V = 307.09 $Å^3$
Z = 2
Density (calc.) = 3.393 g/cm^3

Figures of merit
F_{30} = 110.8(.0087, 31)
M_{20} = 151.0

Comments
The structure of $Ca_2ZnSi_2O_7$ was determined by Warren and Trautz (#1).
The temperature of data collection was approximately 25.0°C.

Additional patterns
PDF card 12-453

Reference
#1. Warren, B.E. and Trautz, O.R.
Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.(1930) 75,525.

d(Å)	I^{rel}	hkl	2θ(°)
5.533	1L	1 1 0	16.005
5.016	15	0 0 1	17.668
4.222	7	1 0 1	21.026
3.911	1L	2 0 0	22.718
3.716	38	1 1 1	23.928
3.500	4	2 1 0	25.431
3.086	63	2 0 1	28.910
2.871	100	2 1 1	31.130
2.767	13	2 2 0	32.332
2.508	8	0 0 2	35.770
2.475	36	3 1 0	36.274
2.423	13	2 2 1	37.080
2.388	7	1 0 2	37.638
2.3143	8	3 0 1	38.883
2.2843	5	1 1 2	39.414
2.2195	8	3 1 1	40.615
2.1711	1L	3 2 0	41.563
2.1113	1	2 0 2	42.797
2.0389	14	2 1 2	44.396
1.9564	2	4 0 0	46.375
1.8985	6	4 1 0	47.874
1.8585	11	2 2 2	48.973
1.8447	5	3 3 0	49.362
1.8231	3	4 0 1	49.987
1.8079	1L	3 0 2	50.437
1.7757	12	4 1 1	51.417
1.7620	38	3 1 2	51.849
1.7503	19	4 2 0	52.221
1.7316	9	3 3 1	52.827
1.6723	1L	0 0 3	54.855
1.6524	6	4 2 1	55.572
1.6413	3	3 2 2	55.980
1.6351	1L	1 0 3	56.211
1.6006	5	1 1 3	57.536
1.5369	6	2 0 3	60.159
1.5343	5	5 1 0	60.271
1.5133	3	4 1 2	61.199
1.5082	5	2 1 3	61.427
1.4943	1L	4 3 1	62.062
1.4671	8	5 1 1	63.342
1.4526	1L	5 2 0	64.050
1.4346	7	4 2 2	64.952
1.4306	7	2 2 3	65.154
1.4073	3	3 0 3	66.373
1.3954	7	5 2 1	67.012
1.3849	7	3 1 3	67.586
1.3419	1L	5 3 0	70.067
1.3333	4	4 4 1	70.583
1.3274	1L	4 3 2	70.944
1.3243	1L	3 2 3	71.136
1.3088	5	5 1 2	72.111
1.3040	3	6 0 0	72.417
1.2967	1L	5 3 1	72.892
1.2863	1L	6 1 0	73.575
1.2708	2	4 0 3	74.622

continued

Calcium Zinc Silicate, $Ca_2ZnSi_2O_7$ (continued)

d(A)	I^{rel}	hkl			2θ(°)
1.2621	1L	6	0	1	75.230
1.2571	6	5	2	2	75.575
1.2542	6	4	1	3+	75.783
1.2464	2	6	1	1	76.340
1.2387	4	3	3	3	76.904
1.2230	1L	1	1	4	78.074
1.2111	2	4	4	2	78.994
1.2084	1L	4	2	3	79.203
1.2012	4	6	2	1	79.776
1.1874	3	5	4	1	80.892
1.1832	4	5	3	2	81.238
1.1803	1L	2	1	4	81.484
1.1664	1L	6	3	0	82.661
1.1572	3	6	0	2	83.463
1.1445	3	6	1	2	84.600
1.1422	3	2	2	4+	84.816
1.1305	5	5	1	3	85.902
1.1185	3	3	1	4	87.058
1.0986	1	5	4	2	89.037
1.0968	1	5	2	3	89.230

Calcium Zirconium Oxide, $CaZrO_3$

Synonym
Calcium zirconate

CAS registry no.
12013-47-7

Sample
The sample was from Aesar Division of Johnson Matthey Inc., Seabrook, NH.

Color
Colorless

Symmetry classifications

Crystal System	Orthorhombic
Space Group	Pnma (62)
Pearson Symbol	oP20
Structure Type	Distorted perovskite (#1)

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 Å
2θ Standard	Si
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±1

Crystallographic constants of this sample
a = 5.7558 (3) Å
b = 8.0101 (14)
c = 5.5929 (6)

a/b = 0.7186
c/b = 0.6982

V = 257.86 $Å^3$
Z = 4
Density (calc.) = 4.619 g/cm^3

Figures of merit
F_{30} = 97.8(.0088, 35)
M_{20} = 88.8

Comments
There is a cubic form of $CaZrO_3$ stable at 2000°C (#2).
The mean temperature of data collection was 23.2°C.

Additional patterns
PDF card 9-364
Coughanour et al. (#3)

References

#1. Megaw, H.D.
Proc. Phys.-Math. Soc. Jpn.(1946) 58,133.
#2. Foex, M. et al.
C. R. Seances Acad. Sci., Ser. C(1967) 264,1837.
#3. Coughanour, L.W. et al.
J. Res. Natl. Bur. Stand. (U.S.)(1955) 54,191.

d(Å)	I^{rel}	hkl	2θ(°)
4.009	36	1 0 1+	22.155
3.587	2	1 1 1	24.799
2.876	26	2 0 0	31.068
2.834	100	1 2 1	31.540
2.797	23	0 0 2	31.975
2.708	1L	2 1 0	33.050
2.559	1L	2 0 1	35.040
2.515	2	1 0 2	35.674
2.438	2	2 1 1	36.841
2.409	5	0 3 1	37.295
2.400	5	1 1 2	37.437
2.336	4	2 2 0	38.510
2.2927	2	0 2 2	39.265
2.2228	3	1 3 1	40.552
2.1561	2	2 2 1	41.865
2.1294	1L	1 2 2	42.414
2.0051	48	2 0 2	45.184
1.9577	2	2 3 0	46.341
1.9459	2	2 1 2	46.640
1.8480	1L	2 3 1	49.270
1.8306	1	1 3 2	49.770
1.8149	7	3 0 1+	50.228
1.7928	16	2 2 2	50.891
1.7740	4	1 0 3	51.470
1.7702	3	3 1 1	51.591
1.7316	1L	1 1 3	52.826
1.6532	17	3 2 1	55.541
1.6446	15	2 4 0	55.858
1.6282	16	0 4 2	56.471
1.6214	24	1 2 3	56.731
1.5007	1	3 3 1	61.765
1.4392	5	4 0 0	64.721
1.4172	11	2 4 2	65.849
1.3986	2	0 0 4	66.840
1.3542	2	4 2 0	69.336
1.3451	3	3 4 1	69.875
1.3275	1L	1 4 3	70.935
1.2680	8	3 2 3	74.816

Cesium Hydrogen Phosphate, CsH_2PO_4

Synonym
Cesium dihydrogen orthophosphate

CAS registry no.
18649-05-3

Sample
CsH_2PO_4 was precipitated by adding ethanol to stoichiometric amounts of Cs_2CO_3 and H_3PO_4 in water solution.

Color
Colorless

Symmetry classifications

Crystal System	Monoclinic
Space Group	$P2_1/m$ (11)
Pearson Symbol	mP16

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	W
Scanned to	4.0° 2θ
$\sigma(I^{rel})$	±4

Crystallographic constants of this sample
a = 7.9072 (9) A
b = 6.3869 (9)
c = 4.8792 (7)
β = 107.712 (11)°

a/b = 1.2380
c/b = 0.7639

V = 234.73 A^3
Z = 2
Density (calc.) = 3.253 g/cm^3

Figures of merit
F_{30} = 58.5(.0095, 54)
M_{20} = 44.9

Comments
The structure was qualitatively determined by Uesu and Kobayashi (#1).
A tetragonal form (#2) and an orthorhombic form (#3) have also been reported.
The temperature of data collection was approximately 25.0°C.

References

#1. Uesu, Y. and Kobayashi, J.
Phys. Status Solidi A(1976) 34,475.
#2. Rez, I.S. et al.
Izv. Akad. Nauk SSSR, Ser. Fiz.(1967) 31,1082.
#3. Fellner-Feldeff, H.
Tschermaks Mineral. Petrogr. Mitt. (1952) 3, 37.

d(A)	I^{rel}	hkl	2θ(°)
4.868	16	1 1 0	18.209
4.644	8	0 0 1	19.095
3.760	100	0 1 1	23.641
3.509	7	1 0 1	25.365
3.489	14	-2 0 1	25.507
3.194	21	0 2 0	27.911
3.074	43	1 1 1	29.029
2.939	6	1 2 0	30.394
2.632	12	0 2 1+	34.038
2.569	9	2 0 1	34.890
2.510	2	3 0 0	35.747
2.436	26	2 2 0	36.866
2.376	22	-3 1 1	37.829
2.357	15	-2 2 1	38.158
2.337	18	3 1 0	38.490
2.324	14	0 0 2	38.712
2.278	8	-1 1 2	39.519
2.1841	5	0 1 2	41.304
2.0479	5	1 3 0	44.189
2.0011	5	2 2 1	45.279
1.9727	5	3 0 1+	45.970
1.9660	6	-4 0 1	46.134
1.9544	3	1 1 2	46.425
1.9462	8	-3 1 2	46.631
1.9346	8	-1 3 1+	46.928
1.8844	14	3 1 1	48.257
1.8786	14	-4 1 1+	48.415
1.8201	7	1 3 1	50.077
1.8055	2	4 1 0	50.509
1.7537	4	2 0 2	52.111
1.7453	3	-4 0 2	52.380
1.7265	2	1 2 2	52.994
1.6908	3	2 1 2	54.206
1.6788	1	3 2 1	54.625
1.6746	2	-4 2 1	54.773
1.6364	7	-3 3 1	56.165
1.6227	8	4 2 0	56.680
1.6039	4	-1 3 2	57.405
1.5962	3	0 4 0	57.710
1.5806	2	-5 0 1	58.333
1.5680	5	-2 3 2+	58.849
1.5495	2	0 0 3	59.619
1.5382	12	4 1 1	60.103
1.5348	11	-5 1 1	60.251
1.5107	2	0 4 1	61.315
1.5060	3	0 1 3+	61.526
1.5019	5	-3 1 3	61.711
1.4938	2	3 0 2	62.086
1.4772	4	1 3 2	62.862
1.4743	5	-3 3 2	62.999
1.4705	6	2 4 0	63.178
1.4666	5	5 1 0	63.367
1.4542	2	3 1 2	63.973
1.4484	6	-5 1 2	64.260
1.4446	5	-4 3 1	64.445

continued

Cesium Hydrogen Phosphate, CsH_2PO_4 (continued)

d(A)	I^{rel}	hkl			2θ(°)
1.4338	2	1	0	3	64.995
1.4205	2	4	2	1	65.678
1.4170	1	-5	2	1	65.860
1.3992	1	1	1	3	66.805
1.3945	4	-4	1	3+	67.063
1.3559	2	2	4	1	69.235
1.3531	2	3	2	2+	69.403

Chromium Carbide, Cr_3C_2

Synonym
Trichromium dicarbide

CAS registry no.
12012-05-0

Sample
The sample was obtained from Aesar Division of Johnson Matthey, Inc., Seabrook, NH.

Color
Dark gray

Symmetry classifications

Crystal System	Orthorhombic
Space Group	Pnam (62)
Pearson Symbol	oP20
Structure Type	Cr_3C_2

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±3

Crystallographic constants of this sample

a = 5.5273 (2) A
b = 11.4883 (5)
c = 2.8286 (2)

a/b = 0.4811
c/b = 0.2462

V = 179.61 A^3
Z = 4
Density (calc.) = 6.657 g/cm^3

Figures of merit
F_{30} = 122.2(.0057, 43)
M_{20} = 138.8

Comments
The structure was determined by Hellbom and Westgren (#1). It was refined by Rundquist and Runnsjo (#2). The mean temperature of data collection was 24.0°C.

Additional patterns
PDF card 14-406
Hellbom and Westgren (#1)

References

#1. Hellbom, K. and Westgren, A. Sven. Kem. Tidskr.(1933) 45,141.
#2. Rundquist, S. and Runnsjo, G. Acta Chem. Scand.(1969) 1191,23.

d(A)	I^{rel}	hkl	2θ(°)
4.978	1L	1 1 0	17.804
3.983	1L	1 2 0	22.302
3.146	2	1 3 0	28.343
2.7460	18	0 1 1	32.582
2.5478	23	1 4 0	35.196
2.4897	13	2 2 0	36.045
2.4596	9	1 1 1	36.502
2.3063	100	1 2 1	39.023
2.2751	10	0 3 1	39.580
2.2409	60	2 3 0	40.210
2.1215	21	1 5 0	42.580
2.1036	10	1 3 1	42.961
1.9912	25	2 4 0	45.518
1.9481	45	2 1 1	46.582
1.9151	29	0 6 0	47.434
1.8934	34	1 4 1	48.011
1.8691	49	2 2 1	48.676
1.8190	27	3 1 0	50.107
1.7833	26	0 5 1	51.182
1.7670	1	2 5 0	51.691
1.7567	8	2 3 1	52.016
1.6975	25	1 5 1	53.972
1.6602	3	3 3 0	55.289
1.6285	6	2 4 1	56.458
1.5734	5	1 7 0+	58.625
1.5302	9	3 1 1	60.450
1.4987	7	2 5 1	61.858
1.4375	3	3 5 0	64.803
1.4192	3	0 7 1	65.742
1.4143	19	0 0 2	66.004
1.3902	1	1 8 0	67.298
1.3720	5	4 1 0	68.313
1.3273	4	3 6 0	70.951
1.2998	1	4 3 0	72.691
1.2812	2	3 5 1	73.916
1.2626	5	2 7 1	75.192
1.2474	13	1 8 1	76.268
1.2367	5	1 4 2	77.054
1.2342	6	4 1 1	77.234
1.2296	3	2 2 2	77.581
1.2254	8	3 7 0	77.896
1.2135	6	4 2 1	78.806
1.2017	11	3 6 1	79.731
1.1961	12	2 3 2	80.184
1.1810	10	4 3 1	81.421
1.1768	6	1 5 2	81.778
1.1619	6	2 8 1	83.056
1.1590	6	2 9 0	83.303
1.1531	8	2 4 2	83.832
1.1397	4	4 4 1	85.042
1.1377	11	0 6 2	85.225
1.1247	8	1 10 0+	86.451
1.1167	9	3 1 2	87.226
1.1005	4	5 1 0	88.851
1.0923	4	4 5 1	89.693

continued

d(A)	I^{rel}	hkl	2θ(°)
1.0856	1	5 2 0	90.395
1.0767	2	3 3 2	91.354
1.0722	1	2 9 1	91.845
1.06085	3	2 10 0	93.123
1.05708	3	4 7 0	93.556
1.05190	3	2 6 2+	94.158
1.04926	3	3 9 0	94.468
1.03173	3	5 4 0	96.595
1.02616	2	1 11 0	97.295
1.01339	2	5 2 1	98.950

Chromium Carbide, $Cr_{23}C_6$

CAS registry no.
12105-81-6

Sample
The sample was obtained from CERAC, Inc., Milwaukee, WI.

Spectrographic analysis (wt.%, CERAC, Inc.)
0.1 Al, Fe, Si
0.08 Mo
0.07 Mg
0.01 V
0.008 Ti
0.003 Ni
0.002 Ca, Cu

Color
Gray

Symmetry classifications

Crystal System	Cubic
Space Group	Fm3m (225)
Pearson Symbol	cF116

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±1

Crystallographic constants of this sample
a = 10.6599 (5) A

V = 1211.32 A^3
Z = 4
Density (calc.) = 6.953 g/cm^3

Figures of merit
F_{28} = 69.6(.0106, 38)
M_{20} = 114.2

Comments
The structure was determined by Westgren (#1).
The mean temperature of data collection was 24.0°C.

Additional patterns
PDF card 14-407

Reference
#1. Westgren, A.
Jernkontorets Ann.(1933) 17,501.

d(A)	I^{rel}	hkl	2θ(°)
6.148	1	1 1 1	14.395
3.214	1	3 1 1	27.737
3.077	1	2 2 2	28.993
2.666	4	4 0 0	33.591
2.445	1	3 3 1	36.724
2.383	23	4 2 0	37.718
2.176	24	4 2 2	41.461
2.0520	100	5 1 1	44.097
1.8840	20	4 4 0	48.266
1.8016	22	5 3 1	50.625
1.7767	12	6 0 0	51.388
1.6857	2	6 2 0	54.382
1.6261	2	5 3 3	56.552
1.6067	6	6 2 2	57.298
1.4930	1L	5 5 1	62.120
1.4788	1L	6 4 0	62.786
1.3327	2	8 0 0	70.622
1.2928	2	8 2 0	73.146
1.2560	12	8 2 2	75.654
1.2308	6	7 5 1	77.490
1.2227	15	6 6 2	78.096
1.1920	2	8 4 0	80.516
1.1698	4	9 1 1	82.367
1.1174	1	9 3 1	87.160
1.0879	6	8 4 4	90.157
1.0712	3	7 7 1	91.959
1.0452	1L	10 2 0	94.945
1.0259	1	10 2 2	97.322

Chromium Nitride, β-Cr_2N

CAS registry no.
24094-93-7

Sample
The sample was obtained from Aesar Division of Johnson Matthey, Inc., Seabrook, NH.

Color
Dark gray

Symmetry classifications

Crystal System	Hexagonal
Space Group	$P\bar{3}1m$ (162)
Pearson Symbol	hP9
Structure Type	Fe_2N

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±1

Crystallographic constants of this sample
a = 4.8113 (2) A
c = 4.4841 (2)

c/a = 0.9320

V = 89.89 A^3
Z = 3
Density (calc.) = 6.539 g/cm^3

Figures of merit
F_{23} = 61.0(.0075, 50)
M_{20} = 139.1

Comments
The structure was determined by Ericksson (#1). An earlier report had given a close-packed hexagonal cell having one-third the volume of the cell given here.
The mean temperature of data collection was 23.9°C.

Additional patterns
PDF card 27-127

Reference
#1. Ericksson, S.
Jernkontorets Ann.(1934) 118,530.

d(A)	I^{rel}	hkl	2θ(°)
3.052	4	1 0 1	29.238
2.4057	15	1 1 0	37.350
2.2419	21	0 0 2	40.191
2.1201	100	1 1 1	42.611
2.0832	1	2 0 0	43.402
1.8888	1	2 0 1	48.137
1.6405	19	1 1 2	56.012
1.4861	1L	2 1 1	62.439
1.3892	15	3 0 0	67.349
1.2696	13	1 1 3	74.704
1.2030	1L	2 2 0	79.632
1.1808	10	3 0 2	81.441
1.1619	10	2 2 1	83.050
1.1209	2	0 0 4	86.817
1.0600	3	2 2 2	93.222
1.0162	2	1 1 4	98.582
0.93710	4	2 2 3	110.572
0.91424	1L	3 1 3	114.822
0.90922	1L	4 1 0	115.818
0.89104	8	4 1 1	119.650
0.87230	6	3 0 4	124.029
0.84258	4	4 1 2	132.190
0.84032	5	1 1 5	132.889

Chromium Silicide, Y-$CrSi_2$

Synonym
Chromium disilicide

CAS registry no.
12018-09-6

Sample
The sample was obtained from TRG Co., Yonkers, NY.
It contained a small amount of an unknown admixture, possibly Cr_3Si.

Color
Dark gray

Symmetry classifications
Crystal System Hexagonal
Space Group $P6_222$ (180)
Pearson Symbol $hP9$

Data collection and analysis parameters
Radiation $CuK\alpha_1$
Wavelength 1.5405981 A
2θ Standard Ag
Scanned to 5.0° 2θ
$\sigma(I^{rel})$ ±2

Crystallographic constants of this sample
a = 4.4281 (2) A
c = 6.3691 (4)

c/a = 1.4383

V = 108.15 A^3
Z = 3
Density (calc.) = 4.982 g/cm^3

Figures of merit
F_{30} = 60.1(.0135, 37)
M_{20} = 103.1

Comments
The structure was determined by Boren (#1).
The mean temperature of data collection was 21.7°C.

Additional patterns
PDF card 12-596

Reference
#1. Boren, B.
Ark. Kemi Mineral. Geol.(1933) 11A, No.10.

d(A)	I^{rel}	hkl	2θ(°)
3.838	5	1 0 0	23.155
3.289	19	1 0 1	27.093
2.450	11	1 0 2	36.649
2.214	19	1 1 0	40.720
2.123	34	0 0 3	42.555
2.090	100	1 1 1	43.247
1.917	7	2 0 0	47.394
1.8572	1	1 0 3	49.010
1.8363	1L	2 0 1	49.605
1.8174	65	1 1 2	50.155
1.5319	11	1 1 3	60.375
1.4710	2	1 0 4	63.157
1.4224	4	2 0 3	65.578
1.4133	3	2 1 1	66.053
1.3190	2	2 1 2	71.464
1.2928	20	1 1 4	73.145
1.2782	5	3 0 0	74.120
1.2537	21	3 0 1	75.821
1.2088	1L	1 0 5	79.169
1.1972	1L	2 1 3	80.098
1.1866	7	3 0 2	80.960
1.1068	6	2 2 0	88.204
1.1040	8	1 1 5	88.495
1.0953	2	3 0 3	89.382
1.0718	1L	2 1 4	91.899
1.0639	1L	3 1 0	92.783
1.0611	1	2 0 5	93.093
1.0490	1L	3 1 1	94.494
1.0089	1L	3 1 2	99.551
0.9968	2	3 0 4	101.201
0.9817	5	2 2 3	103.371
0.9586	1L	4 0 0	106.943
0.9570	1	2 1 5	107.208
0.9286	1L	2 0 6	112.092
0.9023	3	3 0 5	117.227
0.8844	1L	3 1 4	121.143
0.8738	1L	4 0 3	123.655
0.8715	1L	3 2 1	124.232
0.85637	1L	2 1 6	128.182
0.84798	1L	3 2 2	130.570
0.84157	2	1 1 7	132.500
0.83687	1L	4 1 0	133.983
0.82966	4	4 1 1	136.388

Chromium Tungsten Oxide, Cr_2WO_6

Synonym
Chromium tungstate

CAS registry no.
13765-57-6

Sample
The sample was made by heating a 1:1 molar mixture of Cr_2O_3 and WO_3 at up to 975°C for 3 days with intermittent grinding.

Color
Reddish black

Symmetry classifications

Crystal System	Tetragonal
Space Group	$P4_2/mnm$ (136)
Pearson Symbol	$tP\bar{1}8$
Structure Type	Trirutile (#1)

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±1

Crystallographic constants of this sample
a = 4.57960 (19) A
c = 8.8668 (6)

c/a = 1.9362

V = 185.96 A^3
Z = 2
Density (calc.) = 6.855 g/cm^3

Figures of merit
F_{30} = 101.9(.0074, 40)
M_{20} = 156.6

Comments
The structure of Cr_2WO_6 was studied by Trunov and Kovba (#2).
The mean temperature of data collection was 23.6°C.

Additional patterns
PDF card 13-110

References

#1. Kunnmann, W. et al.
J. Phys. Chem. Solids(1968) 29,1359.
#2. Trunov, V.K. and Kovba, L.M.
Inorg. Mater. (Engl. Transl.)(1966) 2,151.

d(A)	I^{rel}	hkl	2θ(°)
4.434	12	0 0 2	20.008
4.069	35	1 0 1	21.827
3.239	100	1 1 0	27.513
2.615	14	1 1 2	34.258
2.4836	70	1 0 3	36.137
2.2902	16	2 0 0	39.308
2.2174	2	0 0 4	40.656
2.1834	7	1 1 3	41.317
2.0487	3	2 1 0	44.172
2.0349	6	2 0 2	44.488
1.9956	11	2 1 1	45.411
1.8289	4	1 1 4	49.818
1.6834	54	2 1 3	54.461
1.6538	3	1 0 5	55.522
1.6192	14	2 2 0	56.813
1.5925	3	2 0 4+	57.856
1.5211	3	2 2 2	60.852
1.5044	2	3 0 1+	61.600
1.4778	6	0 0 6	62.834
1.4484	10	3 1 0	64.260
1.3763	3	3 1 2	68.071
1.3562	13	3 0 3	69.222
1.3443	10	1 1 6	69.922
1.3409	8	2 1 5	70.125
1.3073	1	2 2 4	72.202
1.2572	2	3 2 1	75.570
1.2415	4	2 0 6	76.699
1.2209	2	1 0 7+	78.240
1.2123	3	3 1 4	78.901
1.1985	1L	2 1 6	79.987
1.1669	7	3 2 3	82.617
1.1569	1	3 0 5	83.496
1.1449	3	4 0 0	84.572
1.1086	1	4 0 2+	88.032
1.1020	2	3 2 4+	88.699
1.0915	5	2 2 6	89.777
1.0793	3	3 3 0	91.070
1.0488	2	3 3 2+	94.520
1.0398	6	4 1 3	95.600
1.0343	6	3 1 6	96.270
1.0241	3	4 2 0	97.560

Cobalt Titanium Oxide, $CoTi_2O_5$

Synonym
Cobalt titanate
Cobalt dititanate

CAS registry no.
12017-04-8

Sample
The sample was prepared using CoO_x (x = 1.39) and TiO_2. After an initial calcine at 800°C for 20 hours, the sample was heated at 1430°C for one hour. During the 1430°C heat treatment, the sample was removed from the furnace and ground at 15 minute intervals.

Color
Very dark olive black

Symmetry classifications

Crystal System	Orthorhombic
Space Group	Bbmm (63)
Pearson Symbol	oC32
Structure Type	pseudobrookite

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 Å
2θ Standard	Si
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample
a = 9.7275 (8) Å
b = 10.0750 (9)
c = 3.7304 (3)

a/b = 0.9655
c/b = 0.3703

V = 365.60 $Å^3$
Z = 4
Density (calc.) = 4.265 g/cm^3

Figures of merit
F_{30} = 77.7(.0104, 37)
M_{20} = 78.1

Comments
The structure was studied by Yamaguchi (#1).
The mean temperature of data collection was 23.1°C.

Additional patterns
PDF card 20-1297

Reference
#1. Yamaguchi, G.
Bull. Chem. Soc. Jpn.(1953) 26,204.

d(Å)	I^{rel}	hkl	2θ(°)
5.037	7	0 2 0	17.592
4.865	31	2 0 0	18.221
3.499	76	2 2 0	25.435
3.481	100	1 0 1	25.566
3.292	11	1 1 1	27.064
2.866	4	1 2 1	31.177
2.763	82	2 3 0	32.375
2.518	3	0 4 0	35.628
2.447	27	3 0 1	36.695
2.431	18	4 0 0	36.953
2.418	34	1 3 1	37.145
2.377	4	3 1 1	37.812
2.237	23	2 4 0	40.289
2.202	10	3 2 1	40.954
2.190	20	4 2 0	41.193
2.0417	1	1 4 1	44.332
1.9777	10	3 3 1	45.846
1.9692	28	4 3 0	46.055
1.8644	47	0 0 2	48.806
1.8612	24	2 5 0	48.896
1.7546	14	3 4 1	52.083
1.7416	5	2 0 2	52.501
1.6997	2	5 1 1	53.897
1.6789	18	0 6 0	54.622
1.6454	4	2 2 2	55.827
1.6317	29	5 2 1	56.338
1.6206	5	6 0 0	56.758
1.6006	7	6 1 0	57.535
1.5869	5	2 6 0	58.080
1.5558	13	3 5 1	59.354
1.5519	9	4 5 0	59.520
1.5459	28	2 3 2	59.775
1.5343	23	5 3 1	60.271
1.5123	11	1 6 1	61.241
1.4987	3	0 4 2	61.857
1.4798	5	4 0 2	62.738
1.4602	4	6 3 0	63.677
1.4321	8	2 4 2	65.077
1.4233	7	5 4 1	65.530
1.4196	11	4 2 2	65.722
1.3850	11	3 6 1	67.583
1.3814	10	4 6 0	67.784
1.3542	13	4 3 2	69.337
1.3301	3	1 7 1	70.776
1.3176	4	2 5 2	71.550
1.3106	1	5 5 1	71.996
1.3020	1	7 0 1	72.546
1.2917	6	7 1 1	73.216
1.2633	4	6 5 0	75.142
1.2607	10	7 2 1	75.326
1.2479	10	0 6 2	76.237
1.2335	3	1 0 3	77.286
1.2237	3	6 0 2	78.026
1.2149	4	6 1 2	78.695
1.2086	3	2 6 2	79.187

continued

Cobalt Titanium Oxide, $CoTi_2O_5$ (continued)

d(A)	I^{rel}	hkl	2θ(°)
1.1821	3	8 2 0	81.334
1.1665	2	6 6 0	82.655
1.1610	2	3 0 3	83.135
1.1581	5	1 3 3	83.385
1.1498	2	6 3 2	84.128
1.1185	4	4 8 0	87.053
1.1095	5	2 7 2	87.940
1.0975	5	3 3 3	89.158
1.0939	5	7 5 1	89.526

Copper Arsenic Sulfide, Cu_3AsS_4

Mineral name
Enargite, syn
Wurtzite Group
Related structures Subgroup

Synonym
Copper thioarsenate

CAS registry no.
12336-85-5

Sample
The specimen (NMNH #C849) from Montana was obtained from the National Museum of Natural History, Washington, DC.

Color
Metallic gray

Symmetry classifications

Crystal System	Orthorhombic
Space Group	$Pnm2_1$ (31)
Pearson Symbol	oP16

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	Si FP
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample
a = 6.4367 (5) A
b = 7.4039 (6)
c = 6.1529 (5)

a/b = 0.8694
c/b = 0.8310

V = 293.23 A^3
Z = 2
Density (calc.) = 4.460 g/cm^3

Figures of merit
F_{30} = 42.1(.0099, 72)
M_{20} = 44.6

Comments
The structure was determined by Pauling and Weinbaum (#1) and later confirmed by Kogu and Takane (#2).
The structure is closely related to wurtzite, the hexagonal form of ZnS.
Two other forms of Ca_3AsS_4 have been reported, a tetragonal form (luzonite) by Gaines (#3), and a cubic form by Sclar and Drovenik (#4).
The temperature of data collection was approximately 25.0°C.

Additional patterns
PDF card 10-437
Wernick and Benson (#5)

References
#1. Pauling, L. and Weinbaum, S.
Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.(1934) 88,48.
#2. Kogu, S. and Takane, K.
Proc. Imp. Acad. (Tokyo)(1935) 11,421.
#3. Gaines, R.V.
Am. Mineral.(1957) 42,766.
#4. Sclar, C.B. and Drovenik, M.
Geol. Soc. Am. Bull.(1960) 71,1970.
#5. Wernick, J.H. and Benson, K.E.
J. Phys. Chem. Solids(1957) 3,157.

d(A)	I^{rel}	hkl	2θ(°)
6.434	2L	1 0 0	13.752
4.859	3	1 1 0	18.242
4.734	2	0 1 1	18.729
3.219	100	2 0 0	27.689
3.208	100	1 2 0	27.785
3.076	41	0 0 2	29.006
2.952	4	2 1 0	30.247
2.846	83	1 2 1	31.412
2.660	2	2 1 1	33.662
2.430	2L	2 2 0	36.968
2.258	2L	2 2 1	39.890
2.222	26	1 2 2	40.577
2.0604	2	3 1 0	43.908
1.9541	2	3 1 1+	46.432
1.8567	72	3 2 0	49.022
1.8514	62	0 4 0	49.173
1.7295	25	2 0 3	52.898
1.7285	48	1 2 3	52.928
1.7084	2L	1 4 1	53.602
1.6187	2	3 3 0	56.832
1.6096	6	4 0 0	57.185
1.6045	11	2 4 0	57.383
1.5894	33	3 2 2	57.978
1.5856	33	0 4 2	58.129
1.5666	2	2 2 3+	58.905
1.5569	7	4 0 1	59.310
1.5528	11	2 4 1	59.479
1.5386	2L	0 0 4	60.088
1.4258	6	4 0 2	65.404
1.4230	6	2 4 2	65.545
1.3478	2L	4 3 0	69.712
1.2661	11	4 0 3	74.950
1.2636	12	2 4 3	75.125
1.2190	2L	3 5 0	78.383
1.2158	6	5 2 0	78.632
1.2139	6	0 1 5	78.775
1.1926	8	5 2 1+	80.467
1.1888	7	1 6 1	80.775
1.1846	2L	3 2 4	81.121
1.1489	7	1 2 5	84.210
1.1296	2	4 4 2	85.987

Copper Iron Sulfide, $CuFeS_2$

Mineral name
Chalcopyrite
Chalcopyrite Group
Chalcopyrite Subgroup

CAS registry no.
1308-56-1

Sample
The specimen (NMNH #3009) from Merkur Mines, Germany, was obtained from the National Museum of Natural History, Washington, DC.

Color
Metallic yellow

Symmetry classifications

Crystal System	Tetragonal
Space Group	$I\bar{4}2d$ (122)
Pearson Symbol	tI16

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	4.0° 2θ
$\sigma(I^{rel})$	±4

Crystallographic constants of this sample
a = 5.2893 (4) A
c = 10.423 (2)

c/a = 1.9706

V = 291.60 A^3
Z = 4
Density (calc.) = 4.180 g/cm^3

Figures of merit
F_{21} = 31.1(.011 , 61)
M_{20} = 72.3

Comments
The structure of chalcopyrite was determined by Burdick and Ellis (#1) and refined by Pauling and Brockway (#2).
The mean temperature of data collection was 24.1°C.

Additional patterns
PDF card 9-423
PDF card 25-288

References
#1. Burdick, C.L. and Ellis, J.H.
J. Am. Chem. Soc.(1917) 39,2518.
#2. Pauling, L. and Brockway, L.O.
Z. Kristallogr.(1932) 82,188.

d(A)	I^{rel}	hkl	2θ(°)
4.715	1	1 0 1	18.806
3.038	100	1 1 2	29.372
2.644	5	2 0 0	33.874
2.606	2	0 0 4	34.385
2.308	1L	2 1 1	38.991
1.8697	22	2 2 0	48.660
1.8570	37	2 0 4	49.015
1.5927	27	3 1 2	57.848
1.5753	14	1 1 6	58.547
1.5193	1	2 2 4	60.929
1.3219	3	4 0 0	71.283
1.3027	1L	0 0 8	72.501
1.2125	3	3 3 2	78.881
1.2052	5	3 1 6	79.457
1.1998	3	3 2 5	79.889
1.1789	1L	4 0 4	81.597
1.0770	5	4 2 4	91.327
1.0452	1L	3 2 7	94.951
1.0173	4	5 1 2	98.433
1.0128	5	3 3 6	99.027
0.9351	2	4 4 0	110.923

Hydroxylamine Hydrochloride, $NH_2OH \cdot HCl$

Synonym
Amine hydroxide hydrogen chloride
Oxammonium hydrochloride
Hydroxylammonium chloride

CAS registry no.
5470-11-1

Sample
The sample was obtained from the City Chemical Co., New York City, NY. It was recrystallized from ethanol.

Color
Colorless

Symmetry classifications

Crystal System	Monoclinic
Space Group	$P2_1/n$ (14)
Pearson Symbol	mP28

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	4.0° 2θ
$\sigma(I^{rel})$	±4

Crystallographic constants of this sample
a = 7.2883 (10) Å
b = 5.9473 (10)
c = 6.9546 (10)
β = 114.143 (10)°

a/b = 1.2255
c/b = 1.1694

V = 275.08 A^3
Z = 4
Density (calc.) = 1.678 g/cm^3

Figures of merit
F_{30} = 43.1(.0151, 46)
M_{20} = 34.3

Comments
The structure was determined by Jerslev (#1).
The temperature of data collection was approximately 25.0°C.

Additional patterns
PDF card 26-488

Reference
#1. Jerslev, B.
Acta Crystallogr.(1948) 1,21.

d(A)	I^{rel}	hkl	2θ(°)
5.98	1	-1 0 1	14.811
4.435	3	1 1 0	20.005
4.340	4	0 1 1	20.446
4.215	4	-1 1 1	21.059
3.870	7	1 0 1	22.963
3.240	22	1 1 1	27.505
3.170	3	0 0 2	28.125
3.086	3	-2 1 1	28.906
2.986	100	-2 0 2	29.895
2.904	70	2 1 0	30.761
2.801	62	0 1 2	31.924
2.717	10	1 2 0	32.943
2.694	20	0 2 1	33.224
2.668	3	-2 1 2	33.557
2.423	5	-3 0 1	37.066
2.357	9	1 2 1	38.146
2.342	15	2 1 1	38.406
2.299	13	1 1 2	39.147
2.258	4	-1 2 2	39.888
2.244	5	-3 1 1	40.147
2.152	5	-1 1 3	41.957
2.106	11	-2 2 2	42.907
1.993	6	0 1 3	45.467
1.935	7	2 2 1+	46.920
1.900	2	1 3 0	47.831
1.888	3	-3 1 3	48.155
1.880	6	-1 3 1	48.366
1.869	4	3 0 1	48.690
1.840	4	2 1 2	49.487
1.826	2	-3 2 2	49.900
1.814	3	1 0 3	50.268
1.7938	3	-2 2 3	50.862
1.7827	5	3 1 1	51.200
1.7344	1L	1 1 3	52.734
1.7298	14	-4 1 2	52.886
1.7211	8	-1 3 2+	53.174
1.6628	15	4 0 0	55.194
1.6208	1	-4 1 3+	56.754
1.6015	1	4 1 0	57.498
1.5863	2	0 0 4	58.105
1.5825	2	3 2 1	58.258
1.5646	8	2 3 1	58.988
1.5479	1L	1 2 3	59.686
1.5326	2	0 1 4	60.346
1.4926	4	-4 0 4	62.139
1.4767	1L	2 1 3	62.885
1.4651	1	-4 2 3	63.438
1.4508	3	1 4 0+	64.141
1.4466	7	0 3 3	64.345
1.4238	3	-5 0 1	65.504
1.4160	1L	-5 1 2	65.914
1.4049	1L	-3 3 3	66.502
1.3997	1L	0 2 4	66.781
1.3850	2	-5 1 1+	67.585
1.3789	1	-5 1 3+	67.925

continued

d(A)	I^{rel}	hkl			2θ(°)
1.3752	2	-2	4	1	68.131
1.3688	1L	-3	0	5	68.495
1.3662	1	-1	4	2	68.642
1.3603	1	3	3	1	68.982
1.3571	3	2	4	0+	69.166
1.3532	2	-1	0	5	69.396
1.3378	1L	1	3	3	70.313
1.3320	3	-4	3	1	70.663
1.3158	2	4	2	1	71.664

Iron Carbide, Fe_3C

Mineral name
Cohenite, syn

Synonym
Cementite

CAS registry no.
12011-66-4

Sample
The sample was obtained from CERAC, Inc., Milwaukee, WI.

Spectrographic analysis (wt.%, CERAC, Inc.)
0.03 Al

Color
Dark grayish brown

Symmetry classifications

Crystal System	Orthorhombic
Space Group	Pnma (62)
Pearson Symbol	oP16

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Ag
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±3

Crystallographic constants of this sample
a = 5.0910 (3) A
b = 6.7434 (4)
c = 4.5260 (2)

a/b = 0.7550
c/b = 0.6712

V = 155.38 A^3
Z = 4
Density (calc.) = 7.675 g/cm^3

Figures of merit
F_{30} = 154.4(.0053, 37)
M_{20} = 233.3

Comments
The structure was determined by Hendricks (#1) and confirmed by Meinhardt and Krisement (#2).
The mean temperature of data collection was 22.7°C.

Additional patterns
PDF card 23-1113
PDF card 34-1

References
#1. Hendricks, S.B.
Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.(1930) 74,534.
#2. Meinhardt, D. and Krisement
Arch. Eisenhuettenwes.(1962) 33,493.

d(A)	I^{rel}	hkl	2θ(°)
3.372	4	0 2 0	26.411
3.024	3	1 1 1	29.514
2.5452	4	2 0 0	35.234
2.3882	43	1 2 1	37.634
2.3815	41	2 1 0	37.744
2.2631	22	0 0 2	39.799
2.2186	22	2 0 1	40.633
2.1074	57	2 1 1	42.880
2.0678	67	1 0 2	43.743
2.0313	56	2 2 0	44.570
2.0132	100	0 3 1	44.993
1.9770	53	1 1 2	45.862
1.8792	5	0 2 2	48.399
1.8723	32	1 3 1	48.589
1.8534	43	2 2 1	49.116
1.7631	19	1 2 2	51.814
1.6914	5	2 0 2	54.185
1.6852	15	2 3 0+	54.399
1.6406	8	2 1 2	56.006
1.5890	19	3 0 1	57.994
1.5789	2	2 3 1	58.400
1.5466	5	3 1 1	59.745
1.5216	2	1 3 2	60.826
1.5118	8	2 2 2	61.262
1.5082	6	1 4 1	61.425
1.4372	1	3 2 1	64.818
1.4143	3	1 1 3	66.003
1.4057	6	2 4 0	66.459
1.3514	4	2 3 2	69.503
1.3426	2	2 4 1	70.022
1.3293	17	1 2 3	70.826
1.2978	2	2 0 3+	72.815
1.2927	3	0 5 1	73.149
1.2593	5	3 2 2	75.423
1.2527	3	0 3 3+	75.891
1.2253	14	4 0 1	77.903
1.2162	16	1 3 3	78.595
1.2054	2	4 1 1	79.438
1.1940	3	2 4 2	80.351
1.1918	11	2 5 0	80.535
1.1622	20	3 3 2	83.026
1.1563	1	3 4 1	83.550
1.1524	15	2 5 1	83.895
1.1315	6	0 0 4	85.809
1.1296	12	1 5 2	85.984
1.1276	12	3 0 3	86.181
1.1238	9	0 6 0+	86.540
1.1121	2	3 1 3	87.685
1.1076	11	4 3 0	88.132

Iron Silicide, $FeSi_2$

Mineral name
Ferdisilicite, syn

Synonym
Iron disilicide

CAS registry no.
12022-99-0

Sample
The sample was obtained from CERAC, Inc. Milwaukee, WI. It contained some FeSi.

Color
Dark gray

Symmetry classifications

Crystal System	Tetragonal
Space Group	P4/mmm (123)
Pearson Symbol	tP3

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	W
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±4

Crystallographic constants of this sample
a = 2.69392 (2) A
c = 5.1361 (3)

c/a = 1.9066

V = 37.27 A^3
Z = 1
Density (calc.) = 4.990 g/cm^3

Figures of merit
F_{27} = 59.1(.0117, 39)
M_{20} = 158.5

Comments
The structure was determined by Aronsson (#1).
An orthorhombic low temperature phase, stable below 915°C, was observed by Bucksch (#2).
The mean temperature of data collection was 24.8°C.

Additional Patterns
PDF card 22-1113

References
#1. Aronsson, B.
Acta Chem. Scand. (1960) 14, 1414.
#2.Bucksch, R.
Z. Naturforsch., A (1967), 22, 2124.

d(A)	I^{rel}	hkl	2θ(°)
5.136	39	0 0 1	17.252
2.694	2	1 0 0	33.229
2.386	59	1 0 1	37.668
1.9046	51	1 1 0	47.712
1.8586	100	1 0 2	48.969
1.7852	12	1 1 1	51.124
1.7123	11	0 0 3	53.471
1.5302	1L	1 1 2	60.448
1.4446	3	1 0 3	64.446
1.3469	12	2 0 0	69.764
1.3032	3	2 0 1	72.468
1.2843	6	0 0 4	73.707
1.2731	10	1 1 3	74.466
1.1730	6	2 1 1	82.095
1.0909	1	2 1 2	89.835
1.0648	6	1 1 4	92.678
1.0586	4	2 0 3	93.379
0.9854	2	2 1 3	102.836
0.9598	2	1 0 5	106.747
0.9524	2	2 2 0	107.959
0.9293	4	2 0 4	111.974
0.8845	1L	3 0 1	121.124
0.87863	1L	2 1 4	122.495
0.85182	2	3 1 0	129.459
0.84764	3	3 0 2	130.669
0.83239	3	2 2 3	135.458
0.81579	1L	1 0 6	141.551

Lead Zirconium Oxide, $PbZrO_3$

Synonym
Lead zirconate

CAS registry no.
12060-01-4

Sample
The sample was made by heating PbO and ZrO_2 together at 900°C overnight.

Color
Gray yellow

Symmetry classifications

Crystal System	Orthorhombic
Space Group	P2cb (32)
Pearson Symbol	oP40

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	4.0° 2θ
$\sigma(I^{rel})$	±1

Crystallographic constants of this sample
a = 8.2318 (13) A
b = 11.7764 (13)
c = 5.8816 (7)

a/b = 0.6990
c/b = 0.4994

V = 570.17 A^3
Z = 8
Density (calc.) = 8.071 g/cm^3

Figures of merit
F_{30} = 44.0(.0093, 73)
M_{20} = 30.5

Comments
Distorted perovskite type (#1,#2). Earlier this phase was considered tetragonal (#3).
Above about 150°C $PbZrO_3$ is cubic, perovskite type (#4).
The temperature of data collection was approximately 25.0°C.

References

#1. Sawaguchi, E. et al.
Phys. Rev.(1951) 83,1078.
#2. Jona, F. et al.
Phys. Rev.(1957) 105,849.
#3. Megaw, H.D.
Proc. Phys. Soc., London(1946) 58,133.
#4. Shirane, G. and Hoshino, S.
Acta Crystallogr.(1954) 7,203.

d(A)	I^{rel}	hkl	2θ(°)
5.265	2	0 1 1	16.825
4.163	8	0 2 1	21.325
4.119	5	2 0 0	21.559
3.269	3	0 3 1	27.261
3.241	4	2 1 1	27.498
2.944	66	0 4 0	30.337
2.927	100	2 2 1	30.519
2.852	4	0 1 2	31.335
2.630	1L	0 2 2	34.059
2.559	1L	2 3 1	35.041
2.510	1L	1 4 1	35.751
2.395	14	2 4 0	37.523
2.354	2	0 3 2	38.201
2.346	3	2 1 2	38.338
2.2162	1L	2 2 2	40.678
2.0807	24	0 4 2	43.458
2.0580	14	4 0 0	43.962
2.0431	2	2 3 2	44.298
1.9342	2	0 1 3	46.937
1.9006	1L	3 4 1	47.820
1.8617	2	0 6 1	48.883
1.8573	2	2 4 2	49.005
1.8444	2	4 2 1	49.372
1.8142	1L	1 2 3	50.249
1.7861	1L	3 3 2	51.098
1.7715	1L	2 6 0	51.548
1.7537	3	0 3 3	52.111
1.7502	4	2 1 3	52.224
1.6963	30	2 6 1	54.016
1.6863	18	4 0 2+	54.362
1.6682	1	4 1 2	55.001
1.6137	2	2 3 3	57.026
1.6016	1L	1 6 2	57.496
1.5488	1L	4 3 2	59.650
1.5067	1L	0 5 3	61.496
1.4721	5	0 8 0	63.101
1.4631	9	4 4 2	63.536
1.4149	1	2 5 3	65.968
1.4086	1	4 1 3	66.301
1.3870	1L	0 6 3	67.475
1.3802	1	4 2 3	67.853
1.3760	2	2 7 2	68.084
1.3714	2	4 5 2	68.348
1.3680	1L	1 6 3	68.541

Lithium Aluminum Silicate, $LiAlSi_2O_6$

Synonym
ß-spodumene

CAS registry no.
1302-37-0

Sample
The sample was made by heating a 1:1:4 molar mixture of Li_2CO_3, γ-Al_2O_3, and SiO_2 up to 1350°C for a total of 78 hours.

Color
Colorless

Symmetry classifications

Crystal System	Tetragonal
Space Group	$P4_32_12$ (96)
Pearson Symbol	$tP^{4}0$

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	FP Ag
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample
a = 7.5392 (6) A
c = 9.1489 (10)

c/a = 1.2135

V = 520.02 A^3
Z = 4
Density (calc.) = 2.377 g/cm^3

Figures of merit
F_{30} = 63.8(.0087, 54)
M_{20} = 57.1

Comments
The structure of ß-spodumene was determined by Li and Peacor (#1).
There is a complete solid solution between this phase and $LiAlSi_3O_8$ (#2).
The mean temperature of data collection was 23.6°C.

Additional patterns
PDF card 22-408

References
#1. Li, C-T. and Peacor, D.R.
Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.(1968) 126,46.
#2. Skinner, B.J. and Evans, H.T.
Am. J. Sci.(1960) 258A,312.

d(A)	I^{rel}	hkl	2θ(°)
5.825	2	1 0 1	15.199
5.336	1	1 1 0	16.600
4.609	7	1 1 1	19.243
3.913	32	1 0 2	22.704
3.487	100	2 0 1	25.528
3.164	9	2 1 1	28.180
2.714	1L	2 1 2	32.980
2.647	2	1 1 3	33.832
2.384	1L	3 1 0	37.700
2.3034	3	2 2 2	39.074
2.2876	1	0 0 4	39.356
2.2618	3	2 1 3	39.824
2.1896	1	1 0 4	41.195
2.1140	3	3 1 2	42.738
2.1019	2	1 1 4	42.997
2.0901	1	3 2 0	43.251
1.9390	5	3 0 3	46.814
1.9012	4	3 2 2	47.804
1.8931	6	2 1 4	48.020
1.8843	10	4 0 0	48.259
1.8787	9	3 1 3	48.413
1.8289	1L	4 1 0	49.820
1.7431	1	4 0 2	52.452
1.7309	1L	1 1 5	52.851
1.7247	1L	3 2 3	53.056
1.6976	1	4 1 2	53.969
1.6579	2	4 2 1	55.370
1.6462	3	2 0 5	55.801
1.6080	1L	2 1 5	57.244
1.6037	1L	4 0 3	57.413
1.5429	2	3 2 4	59.902
1.5350	1	3 3 3	60.241
1.4944	1L	1 0 6	62.055
1.4795	1	3 0 5	62.753
1.4751	1	4 2 3	62.959
1.4600	1	5 1 1	63.689
1.4541	2	4 0 4	63.974
1.4513	1	3 1 5	64.113
1.4322	2	4 3 2	65.074
1.4286	1	4 1 4	65.261
1.4071	2	5 1 2	66.381
1.4031	2	3 3 4	66.595
1.3839	1	5 2 1	67.646
1.3768	1	3 2 5	68.042

Lithium Aluminum Silicate, $LiAlSi_3O_8$

Sample
The sample was made by heating a 1:1:6 molar mixture of Li_2CO_3, α-Al_2O_3, and SiO_2 up to 1350°C for a total of 85 hours with intermittent grinding.

Color
Colorless

Symmetry classifications

Crystal System	Tetragonal
Space Group	$P4_32_12$ (96)
Pearson Symbol	tP52
Structure Type	β Spodumene type

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 Å
2θ Standards	Ag FP
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±1

Crystallographic constants of this sample
a = 7.5053 (9) Å
c = 9.0701 (14)

c/a = 1.2085

V = 510.91 $Å^3$
Z = 4
Density (calc.) = 3.200 g/cm^3

Figures of merit
F_{30} = 40.0(.0119, 63)
M_{20} = 46.1

Comments
The structure of this phase was determined by Skinner and Evans (#1).
There is a complete solid solution between $LiAlSi_3O_8$ and $LiAlSi_2O_6$ (#1).
The mean temperature of data collection was 23.3°C.

Additional patterns
PDF card 15-27

Reference
#1. Skinner, B.J. and Evans, H.T.
Am. J. Sci.(1960) 258A,312.

d(A)	I^{rel}	hkl	2θ(°)
5.782	2	1 0 1	15.311
5.311	1L	1 1 0	16.680
4.583	9	1 1 1	19.353
3.885	25	1 0 2	22.873
3.467	100	2 0 1	25.671
3.357	1L	2 1 0	26.530
3.148	10	2 1 1	28.324
2.698	1L	2 1 2	33.180
2.628	2	1 1 3	34.093
2.411	1	3 0 1	37.270
2.290	5	2 2 2	39.305
2.268	2	0 0 4	39.717
2.247	3	2 1 3	40.100
2.169	1	1 0 4	41.603
2.102	5	3 1 2	42.991
2.084	2	1 1 4	43.377
2.080	2	3 2 0	43.466
1.9277	5	3 0 3	47.105
1.8920	7	3 2 2	48.050
1.8768	13	4 0 0	48.463
1.8665	8	3 1 3	48.749
1.7346	1	4 0 2	52.730
1.6886	1	4 1 2	54.280
1.6497	3	4 2 1	55.672
1.6402	4	3 1 4	56.022
1.6337	4	2 0 5	56.266
1.5334	1L	3 2 4	60.310
1.5269	1L	3 3 3	60.594
1.4817	1L	1 0 6	62.646
1.4723	1L	5 1 0	63.095
1.4683	1L	3 0 5	63.285
1.4537	2	1 1 6	63.995

Lithium Manganese Oxide, $LiMnO_2$

Synonym
Lithium manganate

CAS registry no.
12162-79-7

Sample
The sample was made by heating a 1:2 molar mixture of Li_2CO_3 and $MnCO_3$ at 900 - 1100°C for 3 days with several intermediate grindings.

Color
Black

Symmetry classifications

Crystal System	Orthorhombic
Space Group	Pmnm (59)
Pearson Symbol	oP8

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	4.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample

a = 4.5756 (4) A
b = 5.7510 (4)
c = 2.8062 (2)

a/b = 0.7956
c/b = 0.4879

V = 73.84 A^3
Z = 2
Density (calc.) = 4.222 g/cm^3

Figures of merit
F_{30} = 105.2(.0073, 39)
M_{20} = 174.8

Comments
The structure was determined by Hoppe et al. (#1).
The mean temperature of data collection was 24.4°C.

Additional patterns
PDF card 9-109
PDF card 23-361
Schmier and Sterr (#2)

References
#1. Hoppe, R. et al.
Z. Anorg. Allg. Chem.(1975) 417,1.
#2. Schmier, A. and Sterr, G.
Naturwissenschaften(1965) 52,392.

d(A)	I^{rel}	hkl	2θ(°)
5.747	80	0 1 0	15.405
3.581	55	1 1 0	24.843
2.522	29	0 1 1	35.570
2.4344	16	1 2 0	36.893
2.3923	15	1 0 1	37.566
2.2880	81	2 0 0	39.349
2.2089	20	1 1 1	40.819
2.1253	10	2 1 0	42.500
2.0086	100	0 2 1	45.102
1.9164	6	0 3 0	47.400
1.8380	1L	1 2 1	49.556
1.7679	3	1 3 0	51.660
1.6947	9	2 1 1	54.070
1.5829	6	0 3 1	58.241
1.5095	55	2 2 1	61.368
1.4960	16	1 3 1	61.984
1.4743	4	3 1 0	62.998
1.4692	5	2 3 0	63.241
1.4377	12	0 4 0	64.795
1.4031	15	0 0 2	66.598
1.3720	1L	1 4 0	68.311
1.3630	3	0 1 2	68.825
1.3474	2	3 2 0	69.737
1.3399	2	3 0 1	70.183
1.3063	9	1 1 2	72.270
1.2323	4	1 4 1	77.376
1.2173	12	2 4 0	78.516
1.1962	11	2 0 2	80.173
1.1711	2	2 1 2	82.259
1.1499	1L	0 5 0	84.116
1.1439	4	4 0 0	84.661
1.1322	2	0 3 2	85.740
1.1156	3	1 5 0	87.335
1.0983	2	3 3 1	89.073

Lithium Manganese Oxide, $LiMn_2O_4$

Sample
The sample was prepared from Li_2CO_3 and $MnCO_3$. The mixture was calcined in air at 700°C for 21 hours, then in air at 825°C for 21 hours.

Color
Blackish blue

Symmetry classifications

Crystal System	Cubic
Space Group	Fd3m (227)
Pearson Symbol	cF56
Structure Type	$MgAl_2O_4$ (spinel) (#1)

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	FP Ag
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±1

Crystallographic constants of this sample
a = 8.24762 (16) A

V = 561.03 A^3
Z = 8
Density (calc.) = 4.281 g/cm^3

Figures of merit
F_{25} = 78.1(.0094, 34)
M_{20} = 197.9

Comments
The mean temperature of data collection was 23.7°C.

Additional patterns
PDF card 18-736

Reference
#1. Wickham, D.J. and Croft, W.J.
Phys. Chem. Solids(1958) 7,351.

d(A)	I^{rel}	hkl	2θ(°)
4.764	100	1 1 1	18.611
2.914	1L	2 2 0	30.651
2.487	38	3 1 1	36.086
2.381	10	2 2 2	37.748
2.0621	33	4 0 0	43.870
1.8921	7	3 3 1	48.048
1.5874	10	5 1 1	58.058
1.4581	16	4 4 0	63.782
1.3941	7	5 3 1	67.081
1.2578	3	5 3 3	75.528
1.2436	3	6 2 2	76.549
1.1905	4	4 4 4	80.637
1.1551	2	5 5 1	83.653
1.0739	2	7 3 1	91.661
1.0310	1	8 0 0	96.680
1.0078	1L	7 3 3	99.695
0.9523	1	7 5 1	107.972
0.9461	1L	6 6 2	109.017
0.92206	1L	8 4 0	113.318
0.90520	1L	9 1 1	116.635
0.86451	1L	9 3 1	126.005
0.84171	1L	8 4 4	132.458
0.82891	1L	7 7 1	136.648
0.79733	1L	9 5 1	150.074
0.79364	1L	10 2 2	152.142

Lithium Titanium Phosphate, $LiTi_2(PO_4)_3$

Synonym
Lithium titanium orthophosphate

Sample
The sample was made by heating a 1:4:6 molar mixture of Li_2CO_3, TiO_2 (anatase), and $(NH_4)H_2PO_4$ at 800°C for 3 days. It contained a small amount of TiP_2O_7.

Color
Colorless

Symmetry classifications

Crystal System	Rhombohedral
Space Group	$R\bar{3}c$ (167)
Pearson Symbol	hR36

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	4.0° 2θ
$\sigma(I^{rel})$	±1

Crystallographic constants of this sample
(Hexagonal axes)
a = 8.5129 (8) A
c = 20.878 (4)

c/a = 2.4525

V = 1310.31 A^3
Z = 6
Density (calc.) = 2.948 g/cm^3

Figures of merit
F_{30} = 54.3(.0076, 73)
M_{20} = 71.1

Comments
Isostructural with other similar double phosphates.
The mean temperature of data collection was 24.2°C (#1).

Additional patterns
PDF card 24-660

References
#1. Masse, P. Bull. Soc. Fr. Mineral Crystallogr. (1970) 93, 500.

d(A)	I^{rel}	hkl	2θ(°)
6.027	13	0 1 2	14.685
4.258	50	1 0 4+	20.844
3.632	100	1 1 3	24.492
3.477	8	2 0 2+	25.600
3.011	28	0 2 4	29.642
2.761	20	2 1 1	32.395
2.694	26	1 1 6+	33.224
2.4569	25	3 0 0+	36.544
2.3180	1	1 2 5	38.818
2.1290	3	2 2 0+	42.422
2.0351	12	2 2 3+	44.482
2.0065	2	3 1 2+	45.152
1.9043	17	1 3 4+	47.720
1.8360	5	3 1 5	49.613
1.8147	16	0 4 2+	50.234
1.7397	2	0 0 12	52.562
1.6862	6	1 3 7+	54.365
1.6706	7	2 1 10	54.915
1.6087	22	4 1 0+	57.220
1.5674	7	4 1 3+	58.873
1.5052	3	0 4 8	61.562
1.4710	2	3 2 7	63.155
1.4602	8	4 1 6+	63.676
1.4188	5	3 3 0+	65.766
1.3900	3	2 4 1+	67.309
1.3811	4	4 2 2	67.801
1.3461	4	2 4 4	69.812
1.3212	6	5 1 1+	71.326
1.3145	2	1 2 14+	71.746
1.2835	5	5 1 4+	73.760
1.2620	3	1 5 5+	75.233
1.2286	5	6 0 0+	77.658
1.2106	1	3 3 9	79.029
1.2039	1	3 4 2	79.562
1.1804	1	5 2 0+	81.470
1.1652	1	2 2 15+	82.770
1.1639	1L	5 2 3+	82.881
1.1592	1L	0 4 14+	83.289
1.1226	1	1 6 1+	86.655
1.1176	1L	6 1 2+	87.145
1.0988	1	1 6 4	89.015
1.0862	2	1 5 11	90.336

Lithium Tungsten Oxide Hydrate, $7Li_2WO_4 \cdot 4H_2O$

Sample
The sample was from City Chemical Co. New York, NY.

Color
Colorless

Symmetry classifications

Crystal System	Cubic
Space Group	$P\bar{4}3m$ (215)
Pearson Symbol	cP61

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample
a = 8.32312 (15) A

V = 576.58 A^3
Z = 1
Density (calc.) = 5.484 g/cm^3

Figures of merit
F_{30} = 178.4(.0054, 31)
M_{20} = 236.0

Comments
The structure of $7Li_2WO_4 \cdot 4H_2O$ was determined by Hullen (#1).
The temperature of data collection was approximately 25.0°C.

Additional patterns
PDF card 13-424 (reported as $Li_2WO_4 \cdot 1/_2H_2O$)
Swanson, H.E., Morris, M.C.; Stinchfield, R.P. and Evans, E.H. (1963). National Bureau of Standards (U.S.) Monogr. 25, 2, 20.
PDF card 22-693 (reported as Li_2WO_4)

Reference
#1. Hullen, A.
Ber. Bunsenges. Phys. Chem.(1966) 70, 598.

d(A)	I^{rel}	hkl	2θ(°)
8.338	47	1 0 0	10.602
5.887	8	1 1 0	15.036
4.807	100	1 1 1	18.442
4.163	15	2 0 0	21.327
3.723	30	2 1 0	23.884
3.398	81	2 1 1	26.205
2.942	30	2 2 0	30.358
2.7738	82	3 0 0	32.247
2.6318	38	3 1 0	34.038
2.5094	9	3 1 1	35.753
2.4025	13	2 2 2	37.402
2.2245	11	3 2 1	40.520
2.0810	11	4 0 0	43.451
2.0184	33	3 2 2	44.870
1.9616	16	3 3 0	46.244
1.9093	37	3 3 1	47.587
1.8611	21	4 2 0	48.900
1.8162	6	4 2 1	50.192
1.7742	4	3 3 2	51.464
1.6990	12	4 2 2	53.922
1.6646	10	4 3 0	55.128
1.6317	5	5 1 0	56.340
1.6021	10	5 1 1	57.476
1.5454	7	5 2 0	59.793
1.5197	20	5 2 1	60.912
1.4713	24	4 4 0	63.143
1.4489	14	4 4 1	64.233
1.4275	10	5 3 0	65.317
1.4069	13	5 3 1	66.395
1.3874	7	6 0 0	67.451
1.3503	8	6 1 1	69.565
1.3161	3	6 2 0	71.649
1.3000	13	5 4 0	72.677
1.2842	2	5 4 1	73.716
1.2692	2	5 3 3	74.737
1.2549	5	6 2 2	75.734
1.2407	7	6 3 0	76.756
1.2275	5	6 3 1	77.739
1.2011	1L	4 4 4	79.780
1.1893	2	7 0 0	80.738
1.1770	3	5 5 0	81.761
1.1654	9	5 5 1	82.749
1.1432	4	7 2 0	84.720
1.1326	7	7 2 1	85.710
1.1120	6	6 4 2	87.686
1.1025	2	7 2 2	88.639
1.0929	5	7 3 0	89.628
1.0837	2	7 3 1	90.600
1.06572	2	6 5 0	92.572
1.05693	4	6 5 1	93.573
1.04064	3	8 0 0	95.500
1.03226	10	6 5 2	96.529
1.02469	6	7 4 1	97.482
1.01677	7	7 3 3	98.505
1.00930	6	6 4 4	99.494
1.00219	3	8 2 1	100.460
0.99477	2	6 5 3	101.492
0.98076	6	6 6 0	103.517
0.97421	2	6 6 1	104.500
0.96765	4	7 5 0	105.509
0.96100	3	7 5 1	106.559
0.95456	2	6 6 2	107.601
0.94850	2	8 3 2	108.608
0.92477	4	9 0 0	112.808
0.91359	6	9 1 1	114.950

continued

Lithium Tungsten Oxide Hydrate, $7Li_2WO_4 \cdot 4H_2O$ (continued)

d(A)	I^{rel}	hkl	2θ(°)
0.90812	4	8 4 2	116.041
0.90288	1	7 6 0	117.113
0.89754	6	7 6 1	118.238
0.88724	1	6 6 4	120.500
0.88228	4	7 6 2	121.637
0.87738	2	9 3 0	122.792
0.87243	3	9 3 1	123.996
0.86300	3	8 5 2	126.400

CAS registry no.
7439-95-4

Sample
The sample was obtained from Fisher Scientific Co. Fair Lawn, NJ. It contained a small amount of $Mg(OH)_2$.

Color
Dark gray

Symmetry classifications

Crystal System	Hexagonal
Space Group	$P6_3/mmc$ (194)
Pearson Symbol	hP2

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	W
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±1

Crystallographic constants of this sample
a = 3.20936 (11) A
c = 5.2112 (3)

c/a = 1.6238

V = 46.48 A^3
Z = 2
Density (calc.) = 1.736 g/cm^3

Figures of merit
F_{27} = 75.6(.0123, 29)
M_{20} = 195.3

Comments
The structure was determined by Jevins et al. (#1). The temperature of data collection was approximately 25.0°C.

Additional patterns
PDF card 4-770, Swanson, H.E. and Tatge, E. (1953). Natl. Bur. Stand. Circ. 539, 1, 10.

Reference
#1. Jevins, A. et al.
Z. Phys. Chem.(1938) 40B,347.

d(A)	I^{rel}	hkl	2θ(°)
2.778	25	1 0 0	32.194
2.605	36	0 0 2	34.399
2.452	100	1 0 1	36.620
1.9002	15	1 0 2	47.829
1.6047	12	1 1 0	57.375
1.4730	16	1 0 3	63.058
1.3899	2	2 0 0	67.314
1.3663	13	1 1 2	68.633
1.3430	8	2 0 1	69.998
1.3028	2	0 0 4	72.495
1.2264	2	2 0 2	77.823
1.1797	2	1 0 4	81.528
1.0854	3	2 0 3	90.415
1.0506	1	2 1 0	94.315
1.0299	4	2 1 1	96.820
1.0116	3	1 1 4	99.187
0.9760	2	1 0 5	104.236
0.9742	2	2 1 2	104.501
0.9505	1L	2 0 4	108.267
0.9266	1	3 0 0	112.477
0.8988	2	2 1 3	117.964
0.87288	2	3 0 2	123.886
0.83381	1	2 0 5	134.986
0.82892	1L	1 0 6	136.646
0.81783	1L	2 1 4	140.739
0.81745	1L	3 0 3	140.890
0.80230	1L	2 2 0	147.525

Magnesium Hydrogen Phosphate Hydrate, $MgHPO_4 \cdot 3H_2O$

Mineral name
Newberyite, syn

Synonym
Magnesium acid orthophosphate

CAS registry no.
14654-11-6

Sample
Precipitated by adding an aqueous solution of $MgSO_4$ to one of Na_2HPO_4 and letting the material stand for 10 days.

Color
Colorless

Symmetry classifications

Crystal System	Orthorhombic
Space Group	Pbca (61)
Pearson Symbol	oP128

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	FP W
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±3

Crystallographic constants of this sample

a = 10.2083 (14) A
b = 10.6845 (15)
c = 10.0129 (15)

a/b = 0.9554
c/b = 0.9371

V = 1092.11 A^3
Z = 8
Density (calc.) = 2.121 g/cm^3

Figures of merit
F_{30} = 66.8(.0112, 40)
M_{20} = 41.9

Comments
The structure was determined by Sutor (#1).
The mean temperature of data collection was 23.5°C.

Additional patterns
PDF card 19-762
PDF card 20-153 (calculated pattern), Swanson, H. E., McMurdie, H. F., Morris, M. C., and Evans, E. H. (1969). Natl. Bur. Stand. (U. S.) Monogr. 25, 7, 139.
Lonsdale and Sutor (#2)

References

#1. Sutor, D. J.
Acta Crystallogr. (1967) 23, 418.
#2. Lonsdale, K. and Sutor, D. J.
Science (Washington, D. C.) (1966) 154, 1353.

d(A)	I^{rel}	hkl	2θ(°)
5.945	52	1 1 1	14.889
5.344	22	0 2 0	16.574
5.109	4	2 0 0	17.345
4.714	47	0 2 1	18.809
4.610	16	2 1 0	19.237
4.498	41	1 0 2	19.721
4.146	33	1 1 2	21.414
3.692	9	2 2 0	24.084
3.652	12	0 2 2	24.350
3.574	11	2 0 2	24.890
3.462	66	2 2 1	25.715
3.437	33	1 2 2	25.900
3.394	2	2 1 2	26.240
3.187	10	1 3 1	27.978
3.086	54	3 1 1	28.911
3.041	100	1 1 3	29.349
2.970	3	2 2 2	30.061
2.815	24	3 0 2	31.765
2.791	22	1 3 2	32.042
2.721	32	3 1 2	32.885
2.704	13	2 1 3	33.100
2.673	3	0 4 0	33.503
2.582	34	0 4 1	34.715
2.553	3	4 0 0	35.120
2.523	11	2 3 2	35.548
2.505	6	0 0 4	35.821
2.501	5	1 4 1	35.881
2.483	4	4 1 0	36.150
2.431	22	1 0 4	36.939
2.409	12	4 1 1	37.295
2.390	13	3 3 1	37.605
2.371	22	1 1 4+	37.920
2.325	1L	3 1 3	38.691
2.304	2	2 4 1+	39.065
2.297	2	1 4 2	39.180
2.275	2	4 0 2	39.577
2.248	1	2 0 4	40.080
2.207	10	3 3 2	40.854
2.199	17	2 1 4+	41.005
2.176	10	3 2 3	41.458
2.139	6	2 4 2	42.212
2.092	8	4 2 2	43.214
2.071	12	2 2 4	43.670
2.0570	5	3 4 1	43.984
2.0433	13	1 4 3	44.294
2.0309	3	4 3 1	44.580
1.9812	9	3 1 4+	45.761
1.9706	3	2 5 0	46.020
1.9295	17	1 5 2+	47.060
1.8958	6	4 2 3	47.947
1.8874	12	3 2 4	48.175
1.8746	10	0 2 5	48.525
1.8351	1	2 5 2	49.640
1.7981	12	1 4 4	50.733
1.7872	6	4 0 4	51.064

continued

Magnesium Hydrogen Phosphate Hydrate, $MgHPO_4 \cdot 3H_2O$ (continued)

d(Å)	I^{rel}	hkl			2θ(°)
1.7626	11	4	1	4+	51.829
1.7542	13	3	3	4	52.095
1.7201	8	2	4	4+	53.207
1.7026	3	3	5	2+	53.800
1.6801	10	6	1	0	54.578
1.6697	9	5	3	2	54.949
1.6588	7	2	6	1	55.339
1.6380	5	4	5	0	56.105
1.6170	1	4	5	1	56.899
1.6053	4	1	5	4	57.351
1.6002	6	6	2	1	57.550
1.5931	10	6	1	2+	57.830
1.5867	12	2	0	6	58.087
1.5655	8	5	1	4+	58.950
1.5566	1	4	5	2	59.322
1.5200	3	2	2	6	60.897
1.5004	2	6	1	3	61.780
1.4922	7	1	7	1	62.156
1.4674	3	6	3	2	63.330
1.4493	4	3	4	5+	64.212
1.4452	8	4	6	1+	64.419
1.4364	1	1	6	4	64.859
1.4152	10	0	4	6	65.957

Magnesium Nitride, Mg_3N_2

CAS registry no.
12057-71-5

Sample

The sample was obtained from CERAC, Inc., Milwaukee, WI. It was run in a dry atmosphere because of its sensitivity to humidity.

Color

Moderate olive brown

Symmetry classifications

Crystal System	Cubic
Space Group	Ia3 (206)
Pearson Symbol	cI80

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±3

Crystallographic constants of this sample

a = 9.9657 (2) A

V = 989.75 A^3
Z = 16
Density (calc.) = 2.709 g/cm^3

Figures of merit

F_{30} = 64.6(.0129, 36)
M_{20} = 68.5

Comments

The structure was determined by von Stackelberg and Paulus (#1).
The mean temperature of data collection was 23.6°C.

Additional patterns

PDF card 1-1289

Reference

#1. von Stackelberg, M. and Paulus, R.
Z. Phys. Chem. (Leipzig)(1933) B22,305.

d(A)	I^{rel}	hkl	2θ(°)
4.987	1	2 0 0	17.771
4.066	25	2 1 1	21.842
3.523	1L	2 2 0	25.259
2.875	44	2 2 2	31.078
2.662	62	3 2 1	33.637
2.490	46	4 0 0	36.036
2.349	1L	4 1 1	38.281
2.228	1	4 2 0	40.452
2.124	60	3 3 2	42.530
2.033	1	4 2 2	44.523
1.954	8	4 3 1	46.429
1.8190	6	5 2 1	50.107
1.7613	100	4 4 0	51.869
1.6165	5	5 3 2	56.917
1.5748	1	6 2 0	58.568
1.5373	7	5 4 1	60.143
1.5018	5	6 2 2	61.717
1.4691	8	6 3 1	63.248
1.4379	7	4 4 4	64.783
1.4094	1	5 4 3	66.259
1.3824	1L	6 4 0	67.728
1.3562	27	7 2 1	69.219
1.3320	1L	6 4 2	70.660
1.2655	18	7 3 2	74.990
1.2456	7	8 0 0	76.401
1.2266	2	5 5 4	77.803
1.1743	1	6 6 0	81.989
1.1431	2	6 6 2	84.736
1.1284	3	7 5 2	86.098
1.1143	3	8 4 0	87.468
1.1006	1L	8 3 3	88.838
1.0746	6	6 5 5	91.586
1.0623	1	6 6 4	92.961
1.0504	2	8 5 1	94.335
1.0279	7	9 3 2	97.074
1.0171	8	8 4 4	98.461
1.0067	3	9 4 1	99.845
0.9966	1L	8 6 0	101.232
0.9868	3	10 1 1	102.631
0.9773	1L	10 2 0	104.027
0.9680	1	9 4 3	105.450
0.9501	4	10 3 1	108.339
0.9333	1	8 7 1	111.248
0.9254	1L	10 4 0	112.687
0.9173	2	10 3 3	114.221
0.9097	1L	10 4 2	115.713
0.9023	1L	9 5 4	117.234
0.8878	5	10 5 1	120.378
0.8809	1	8 8 0	121.958
0.86092	5	9 7 2	126.950
0.85464	1	10 6 0	128.662
0.84829	1L	11 4 1	130.478
0.83631	1	9 6 5	134.166
0.83049	1L	12 0 0	136.105
0.82480	2	9 8 1	138.111

Magnesium Silicide, Mg_2Si

CAS registry no.
22831-39-6

Sample
The sample was obtained from CERAC, Inc., Milwaukee, WI. It contained a small amount of MgO.

Spectrographic analysis (wt.%, CERAC, Inc.)
0.12 Fe
0.05 Al
0.01 Mn
0.001 Ag, Ca, Cr, Cu, Ti

Color
Dark blue

Symmetry classifications
Crystal System Cubic
Space Group Fm3m (225)
Pearson Symbol cF12
Structure Type CaF_2 (#1)

Data collection and analysis parameters
Radiation $CuK\alpha_1$
Wavelength 1.5405981 A
2θ Standard Si
Scanned to 5.0° 2θ
$\sigma(I^{rel})$ ±2

Crystallographic constants of this sample
a = 6.35119 (16) A

V = 256.19 A^3
Z = 4
Density (calc.) = 1.988 g/cm^3

Figures of merit
F_{19} = 140.0(.0071, 19)
M_{19} = 386.5

Comments
There is a high pressure form (#2).
The mean temperature of data collection was 23.7°C.

Additional patterns
PDF card 1-1192

References
#1. Klemm, W. and Westlinning, H.
Z. Anorg. Allg. Chem.(1940) 245,365.
#2. Cannon, P. and Conlin, C.T.
Science (Washington, D.C.)(1964) 145,487.

d(A)	I^{rel}	hkl	2θ(°)
3.668	41	1 1 1	24.242
3.176	12	2 0 0	28.071
2.2456	100	2 2 0	40.122
1.9151	15	3 1 1	47.434
1.8338	2	2 2 2	49.677
1.5881	13	4 0 0	58.030
1.4570	6	3 3 1	63.835
1.4201	3	4 2 0	65.700
1.2965	21	4 2 2	72.903
1.2224	4	5 1 1	78.120
1.1228	4	4 4 0	86.636
1.0736	2	5 3 1	91.698
1.0586	1L	6 0 0	93.380
1.0042	3	6 2 0	100.182
0.96854	1	5 3 3	105.371
0.95754	1L	6 2 2	107.116
0.91669	1	4 4 4	114.345
0.88932	1	5 5 1	120.033
0.88066	1L	6 4 0	122.015

Magnesium Titanium Oxide, $MgTi_2O_5$, form A

Synonyms
Magnesium titanate
Magnesium dititanate

CAS registry no.
12032-35-8

Sample
The sample was prepared from basic magnesium carbonate and TiO_2 by repeated heatings with periodic grinding. Final reaction temperature was 1500°C and the sample was quenched in water.

Color
Gray

Symmetry classifications

Crystal System	Orthorhombic
Space Group	Bbmm (63)
Pearson Symbol	oC32
Structure Type	Pseudobrookite

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	Si FP
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±4

Crystallographic constants of this sample
a = 9.7501 (6) A
b = 9.9802 (6)
c = 3.7483 (3)

a/b = 0.9769
c/b = 0.3756

V = 364.74 A^3
Z = 4
Density (calc.) = 3.644 g/cm^3

Figures of merit
F_{30} = 113.3(.0078, 34)
M_{20} = 117.4

Comments
The structure was studied by Yamaguchi (#1). The lattice parameters change depending upon quenching temperature, with "a", "c", and "V" increasing, and "b" decreasing, with increasing quench temperature (#2). Note a similar pattern for form B, in this publication. A tetragonal phase has been reported (#3). The mean temperature of data collection was 23.9°C.

Additional patterns
PDF card 20-694
Yamaguchi (#1, #4)
Zhdanov and Rusakov (#5)

References

#1. Yamaguchi, G.
Dainippon Yogyo Kyokai Zasshi (J. Jpn. Ceram. Assoc.)(1947) 55,94.
#2. Wechsler, B.A. and Navrotsky, A.
Geol. Soc. Am. Program Annu. Meeting(1982) 14,
#3. Tanaka, Y.
Bull. Chem. Soc. Jpn.(1941) 16,428.
#4. Yamaguchi, G.
Bull. Chem. Soc. Jpn.(1955) 26,204.
#5. Zhdanov, G.S. and Rusakov, A.A.
Dokl. Akad. Nauk SSSR(1952) 82,901.

d(A)	I^{rel}	hkl	2θ(°)
4.989	20	0 2 0	17.763
4.878	32	2 0 0	18.173
4.380	4	2 1 0	20.256
3.499	100	1 0 1	25.437
3.302	5	1 1 1	26.984
2.864	9	1 2 1	31.209
2.748	80	2 3 0	32.560
2.494	1	0 4 0	35.975
2.456	20	3 0 1	36.559
2.4374	9	4 0 0	36.846
2.4108	18	1 3 1	37.268
2.3846	2	3 1 1	37.693
2.3690	2	4 1 0	37.950
2.2213	21	2 4 0	40.580
2.1889	22	4 2 0	41.209
2.0311	2	1 4 1	44.574
1.9753	12	3 3 1	45.904
1.9662	31	4 3 0	46.130
1.8737	38	0 0 2	48.549
1.8471	18	2 5 0	49.295
1.7547	4	0 2 2	52.078
1.7495	20	2 0 2+	52.244
1.7337	3	1 5 1	52.759
1.7295	3	5 0 1	52.895
1.7226	1	2 1 2	53.126
1.7044	4	5 1 1	53.738
1.6638	16	0 6 0	55.157
1.6503	3	2 2 2	55.648
1.6342	18	5 2 1	56.247
1.6252	3	6 0 0	56.584
1.6042	6	6 1 0	57.394
1.5741	5	2 6 0	58.598
1.5482	37	2 3 2+	59.674
1.5443	20	4 5 0	59.842
1.5349	25	5 3 1	60.247
1.5025	8	1 6 1	61.684
1.4986	3	0 4 2	61.862
1.4853	3	4 0 2	62.480
1.4598	5	6 3 0	63.698
1.4321	7	2 4 2	65.077
1.4240	11	4 2 2	65.495
1.3773	7	3 6 1	68.015
1.3739	3	4 6 0	68.202
1.3686	4	2 7 0	68.503
1.3569	13	4 3 2	69.179

continued

d(A)	I^{rel}	hkl			2θ(°)
1.3202	5	1	7	1	71.392
1.3152	10	2	5	2	71.701
1.3072	3	5	5	1	72.212
1.3053	3	7	0	1	72.334
1.2947	6	7	1	1	73.019
1.2633	9	7	2	1	75.142
1.2604	5	6	5	0	75.349
1.2474	2	0	8	0	76.273
1.2439	8	0	6	2	76.526
1.2331	2L	3	7	1	77.322
1.2306	2L	4	7	0	77.508
1.2279	2L	6	0	2	77.709
1.2186	3	6	1	2+	78.416
1.2153	3	7	3	1	78.665
1.2053	4	2	6	2	79.445
1.1839	2	8	2	0	81.178
1.1663	3	3	0	3	82.674
1.1615	3	1	3	3	83.086
1.1586	2	3	1	3	83.346
1.1569	2	7	4	1	83.491
1.1519	3	6	3	2	83.933
1.1123	3	3	8	1	87.660
1.1107	2	4	8	0	87.824
1.1005	3	3	3	3+	88.848

Magnesium Titanium Oxide, $MgTi_2O_5$, form B

Synonym
Magnesium titanate
Magnesium dititanate

CAS registry no.
12032-35-8

Sample
The sample was prepared from basic magnesium carbonate and TiO_2 by repeated heatings with periodic grinding. Final reaction temperature was 1500°C and the sample was quenched in water. To determine whether cell constants change with sample preparation, this sample was then annealed at 700°C for 162 hours, and quenched.

Color
White

Symmetry classifications

Crystal System	Orthorhombic
Space Group	Bbmm (63)
Pearson Symbol	oC32
Structure Type	pseudobrookite

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	Si FP
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±1

Crystallographic constants of this sample
a = 9.7274 (7) A
b = 10.0040 (8)
c = 3.7428 (3)

a/b = 0.9724
c/b = 0.3741

V = 364.22 A^3
Z = 4
Density (calc.) = 3.649 g/cm^3

Figures of merit
F_{30} = 71.5(.0120, 35)
M_{20} = 74.0

Comments
The structure was studied by Yamaguchi (#1). The lattice parameters change depending upon quenching temperature, with "a", "c", and "V" increasing, and "b" decreasing, with increasing quench temperature (#2).
A tetragonal phase is reported (#3).
Note a similar pattern for form A, in this publication.
A tetragonal phase has been reported (#3).
The mean temperature of data collection was 23.7°C.

Additional patterns
PDF card 20-694
Yamaguchi (#1,#4)
Zhdanov and Rusakov (#5)

References

#1. Yamaguchi, G.
Dainippon Yogyo Kyokai Zasshi (J. Jpn. Ceram. Assoc.)(1947) 55,94.
#2. Wechsler, B.A. and Navrotsky, A.
Geol. Soc. Am. Program Annu. Meeting(1982) 14,
#3. Tanaka, Y.
Bull. Chem. Soc. Jpn.(1941) 16,428.
#4. Yamaguchi, G.
Bull. Chem. Soc. Jpn.(1955) 26,204.
#5. Zhdanov, G.S. and Rusakov, A.A.
Dokl. Akad. Nauk SSSR(1952) 82,901.

d(A)	I^{rel}	hkl	2θ(°)
4.998	23	0 2 0	17.730
4.868	24	2 0 0	18.210
4.373	8	2 1 0	20.293
3.493	100	1 0 1	25.479
2.864	9	1 2 1	31.210
2.748	72	2 3 0	32.552
2.450	15	3 0 1	36.652
2.433	10	4 0 0	36.923
2.413	16	1 3 1	37.238
2.380	1L	3 1 1	37.765
2.361	3	4 1 0	38.077
2.224	17	2 4 0	40.536
2.201	1L	3 2 1	40.974
2.187	21	4 2 0	41.237
2.033	2	1 4 1	44.524
1.9748	10	3 3 1	45.918
1.9640	24	4 3 0	46.184
1.8715	29	0 0 2	48.611
1.8510	20	2 5 0	49.183
1.7499	11	3 4 1	52.233
1.7457	10	2 0 2	52.368
1.7358	1	1 5 1	52.690
1.7258	2	5 0 1	53.020
1.7210	2	2 1 2	53.177
1.7008	3	5 1 1	53.860
1.6670	14	0 6 0	55.045
1.6494	1	2 2 2	55.682
1.6323	21	5 2 1	56.318
1.6211	2	6 0 0	56.741
1.6000	5	6 1 0	57.560
1.5774	4	2 6 0	58.461
1.5497	18	3 5 1	59.611
1.5470	28	2 3 2	59.728
1.5330	25	5 3 1	60.330
1.5047	7	1 6 1	61.583
1.4826	5	4 0 2	62.607
1.4672	1L	4 1 2	63.338
1.4583	5	6 3 0	63.770
1.4324	5	2 4 2	65.065
1.4222	12	4 2 2	65.587
1.3785	5	3 6 1	67.946
1.3752	3	4 6 0	68.132
1.3713	3	2 7 0	68.349
1.3550	11	4 3 2	69.289
1.3228	1	1 7 1	71.231

Magnesium Titanium Oxide, $MgTi_2O_5$, form B (continued)

d(Å)	I^{rel}	hkl	2θ(°)
1.3157	8	2 5 2	71.674
1.3073	1	5 5 1	72.202
1.3029	1	7 0 1	72.484
1.2919	5	7 1 1	73.204
1.2606	9	7 2 1	75.331
1.2505	1	0 8 0	76.047
1.2446	9	0 6 2	76.473
1.2376	4	1 0 3	76.987
1.2344	3	3 7 1	77.218
1.2254	1L	6 0 2	77.895
1.2160	3	8 0 0+	78.610
1.2133	3	7 3 1	78.822
1.2062	2	2 6 2	79.380
1.2013	1L	1 2 3	79.765
1.1815	1	8 2 0	81.376
1.1643	1	3 0 3	82.845
1.1626	1	6 6 0	82.995
1.1602	2	1 3 3	83.202
1.1554	1	7 4 1	83.628
1.1504	4	6 3 2	84.076

Manganese Boride, MnB_2

Synonym
Manganese diboride

CAS registry no.
12228-50-1

Sample
The sample was obtained from CERAC, Inc., Milwaukee, WI.

Color
Dark olive

Symmetry classifications

Crystal System	Hexagonal
Space Group	P6/mmm (191)
Pearson Symbol	hP3

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	W
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample
a = 3.00907 (12) A
c = 3.0367 (2)

c/a = 1.0092

V = 23.81 A^3
Z = 1
Density (calc.) = 5.339 g/cm^3

Figures of merit
F_{19} = 86.5(.011 , 20)
M_{19} = 298.6

Comments
The structure was determined by Aronsson and Engstrom (#1).
It contained unidentified impurities with lines at 2.954, 2.435 2.139, 2.013, 1.960, 1.769, 1.285, 1.279, of which 2.435 and 2.139 were the strongest and had relative intensities of 14.
The mean temperature of data collection was 23.4°C.

Additional patterns
PDF card 12-415

Reference
#1. Aronsson, B. and Engstrom, I.
Acta Chem. Scand.(1960) 14,1403.

d(A)	I^{rel}	hkl	2θ(°)
3.038	25	0 0 1	29.380
2.606	76	1 0 0	34.392
1.9782	100	1 0 1	45.834
1.5186	10	0 0 2	60.959
1.5048	22	1 1 0	61.579
1.3482	9	1 1 1	69.691
1.3119	11	1 0 2	71.909
1.3031	6	2 0 0	72.472
1.1975	13	2 0 1	80.066
1.0688	11	1 1 2	92.227
0.9887	4	2 0 2	102.354
0.9851	6	2 1 0	102.886
0.9435	7	1 0 3	109.455
0.9370	12	2 1 1	110.592
0.86860	5	3 0 0	124.955
0.83979	3	1 1 3	133.055
0.83513	3	3 0 1	134.549
0.82626	6	2 1 2	137.585
0.79939	3	2 0 3	148.991

Manganese Silicate, Mn_2SiO_4

Mineral name
Tephroite, syn
Olivine Group
Olivine Subgroup

CAS registry no.
13568-32-6

Sample
The sample was prepared by blending $MnCO_3$ and SiO_2 in a 2:1 molar ratio and heating at 1050°C and 1200°C in a controlled atmosphere with partial pressure of oxygen less than or equal to 10^{-18} atm.

Color
Light gray

Symmetry classifications

Crystal System	Orthorhombic
Space Group	Pmnb (62)
Pearson Symbol	oP28

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	FP W
Scanned to	4.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample
a = 6.2585 (3) A
b = 10.6039 (6)
c = 4.9030 (2)

a/b = 0.5902
c/b = 0.4624

V = 325.39 A^3
Z = 4
Density (calc.) = 4.123 g/cm^3

Figures of merit
F_{30} = 162.3(.0044, 42)
M_{20} = 154.3

Comments
Isostructural with the olivine group of compounds, such as, γ-Ca_2SiO_4 and Fe_2SiO_4 (#1).
A refined structure of Fe_2SiO_4, fayalite, has been reported by Hanke (#2).
The mean temperature of data collection was 22.6°C.

Additional patterns
PDF card 19-788
O'Daniel and Tscheischwili (#1)
Santoro et al. (#3)

References
#1. O'Daniel, H. and Tscheischwili, L.
Z. Kristallogr.(1944) 105,273.
#2. Hanke, K.
Neues Jahrb. Mineral., Monatsh.(1963) 8,192.
#3. Santoro, R.P. et al.
J. Phys. Chem. Solids(1966) 27,655.

d(A)	I^{rel}	hkl	2θ(°)
5.305	9	0 2 0	16.698
4.453	8	0 1 1	19.924
4.047	12	1 2 0	21.946
3.860	9	1 0 1	23.020
3.627	50	1 1 1	24.523
3.599	10	0 2 1	24.714
3.1298	12	2 0 0	28.496
2.8668	92	0 3 1	31.173
2.6946	30	2 2 0	33.221
2.6510	11	0 4 0	33.784
2.6066	69	1 3 1	34.377
2.5597	100	2 1 1	35.027
2.4516	19	0 0 2	36.626
2.4410	17	1 4 0	36.790
2.3890	8	0 1 2	37.621
2.3622	17	2 2 1	38.064
2.3321	16	0 4 1	38.574
2.2314	10	1 1 2	40.390
2.1138	8	2 3 1	42.743
2.0962	4	1 2 2	43.120
2.0226	4	2 4 0	44.772
1.9463	5	0 5 1	46.628
1.9191	1	3 0 1	47.330
1.8890	12	3 1 1	48.131
1.8587	8	1 5 1	48.967
1.8135	72	2 2 2	50.270
1.7999	27	0 4 2	50.678
1.7300	14	1 4 2	52.881
1.7009	16	1 6 0	53.856
1.6871	20	3 3 1	54.334
1.6530	17	2 5 1	55.551
1.6395	9	3 4 0	56.047
1.6155	6	0 1 3	56.955
1.5718	6	3 1 2	58.693
1.5650	33	4 0 0	58.973
1.5540	6	1 5 2	59.431
1.5390	27	2 6 0	60.067
1.5153	2	1 2 3	61.106
1.5007	1	4 2 0	61.767
1.4836	6	0 3 3	62.560
1.4756	1	4 1 1	62.937
1.4476	15	0 7 1	64.299
1.4437	15	1 3 3	64.493
1.4355	12	2 1 3+	64.908
1.4229	1	3 5 1	65.550
1.3976	11	2 2 3+	66.895
1.3910	4	0 4 3	67.250
1.3736	14	4 3 1	68.222
1.3629	3	3 4 2	68.833
1.3583	4	1 4 3	69.100

continued

Manganese Silicate, Mn_2SiO_4 (continued)

d(A)	I^{rel}	hkl			2θ(°)
1.3485	7	3	6	0	69.674
1.3408	2	2	3	3	70.129
1.3190	7	4	0	2	71.463
1.3089	1	4	1	2	72.104
1.3034	6	2	6	2	72.454
1.3001	5	3	6	1	72.671
1.2966	1L	1	8	0	72.893
1.2770	4	3	1	3	74.201
1.2715	4	3	5	2+	74.577
1.2257	6	0	0	4	77.870
1.2197	2	4	5	1	78.330
1.2182	2	5	2	0	78.445
1.2127	1	5	0	1	78.870
1.2091	6	3	3	3	79.149
1.2048	3	5	1	1	79.491
1.1962	9	2	5	3	80.173
1.1914	1	2	7	2	80.563
1.1843	1L	2	8	1	81.146
1.1809	10	4	4	2	81.431
1.1660	3	0	8	2	82.698
1.15750	3	3	4	3	83.439
1.14701	7	5	3	1	84.377
1.13457	1	2	1	4	85.521
1.13214	1	5	4	0	85.749
1.12371	3	4	1	3	86.549
1.11574	8	2	2	4	87.322
1.11264	8	0	4	4	87.628
1.11083	7	0	7	3	87.807
1.10294	1L	5	4	1	88.598
1.09530	1L	1	4	4	89.381
1.09251	1	2	8	2	89.671

Manganese Sulfate, $MnSO_4$

Synonym
Manganous sulfate

CAS registry no.
7785-87-7

Sample
The sample was obtained from the J. T. Baker Chemical Co., Phillipsburg, NJ. It was heated to 400°C overnight.

Color
Pale pink

Symmetry classifications

Crystal System	Orthorhombic
Space Group	Amam (63)
Pearson Symbol	oC24

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	W
Scanned to	4.0° 2θ
$\sigma(I^{rel})$	±1

Crystallographic constants of this sample

a = 6.8447 (5) A
b = 8.0414 (5)
c = 5.2649 (3)

a/b = 0.8512
c/b = 0.6547

V = 289.79 A^3
Z = 4
Density (calc.) = 3.461 g/cm^3

Figures of merit
F_{30} = 114.1(.0069, 38)
M_{20} = 125.2

Comments
The structure was determined by Will et al. (#1). An orthorhombic β-$MnSO_4$ has been reported. The α-β transformation is reported to occur at 438°C on heating and at 328°C on cooling (#2). The mean temperature of data collection was 24.9°C.

Additional patterns
PDF card 11-88

References

#1. Will, G. et al.
Acta Crystallogr.(1965) 19,854.
#2. Kirfel, A. and Will, G.
High Temp. High Pressures(1974) 6,525.

d(A)	I^{rel}	hkl	2θ(°)
4.404	20	0 1 1	20.149
4.020	18	0 2 0	22.092
3.704	72	1 1 1	24.005
3.467	36	1 2 0	25.673
2.703	100	2 1 1	33.115
2.633	29	0 0 2	34.026
2.3885	38	0 3 1	37.629
2.2025	2	0 2 2	40.943
2.0961	6	1 2 2	43.122
2.0869	18	2 0 2	43.322
2.0103	9	0 4 0	45.062
1.9842	6	3 2 0	45.687
1.9592	5	2 3 1	46.303
1.8521	20	2 2 2	49.154
1.7330	11	2 4 0	52.782
1.7112	10	4 0 0	53.507
1.6633	4	1 1 3	55.176
1.6495	4	3 3 1	55.679
1.5976	3	0 4 2	57.654
1.5946	3	4 1 1	57.771
1.5748	5	4 2 0	58.570
1.5557	3	1 4 2	59.357
1.5382	5	0 5 1	60.101
1.5328	7	2 1 3	60.337
1.5009	1	1 5 1	61.758
1.4684	7	0 3 3	63.279
1.4478	15	2 4 2	64.286
1.4360	3	1 3 3	64.879
1.4345	3	4 0 2	64.955
1.4031	2	2 5 1	66.596
1.3911	7	4 3 1	67.246
1.3510	1	4 2 2	69.526
1.3400	1L	0 6 0	70.176
1.3160	3	0 0 4	71.653
1.3084	3	3 4 2	72.134
1.2754	2	3 5 1	74.311
1.2509	1L	0 2 4	76.023
1.2478	1L	2 6 0	76.243
1.2349	1L	3 3 3	77.185
1.2305	1	1 2 4	77.515
1.2112	1L	4 1 3	78.986
1.1944	1L	0 6 2	80.317
1.1859	1L	0 5 3	81.015
1.1766	1L	1 6 2	81.794
1.1679	1L	4 4 2	82.537
1.1628	1L	5 2 2	82.977
1.1439	1	4 5 1	84.661
1.1143	2	4 3 3	87.466
1.1045	1	6 1 1	88.446
1.1012	1	0 4 4	88.777
1.0968	1	3 2 4	89.221

Molybdenum Carbide, α-Mo_2C

CAS registry no.
12069-89-5

Sample
The sample was obtained from CERAC, Inc., Milwaukee, WI. It contained a small percent of MoC.

Spectrographic analysis (wt.%, CERAC, Inc.)
0.1-0.2 Fe, Ni, Si
0.05-0.1 Al, As, Cr, Cu, Mg, Mn, Ti
0.01-0.1 V
0.001 Sn
0.0005-0.005 Ag, Cd

Color
Black

Symmetry classifications
Crystal System Hexagonal
Space Group $P6_3/mmc$ (194)
Pearson Symbol $hP3$
Structure Type Isostructural with W_2C (#1)

Data collection and analysis parameters
Radiation $CuK\alpha_1$
Wavelength 1.5405981 A
2θ Standard Si
Scanned to 5.0° 2θ
$\sigma(I^{rel})$ ±2

Crystallographic constants of this sample
a = 3.0124 (4) A
c = 4.7352 (7)

c/a = 1.5719

V = 37.21 A^3
Z = 1
Density (calc.) = 9.098 g/cm^3

Figures of merit
F_{13} = 78.5(.0127, 13)
M_{13} = 222.3

Comments
An orthorhombic distortion of this form was reported by Christensen (#2).
A cubic form of Mo_2C was formed at high CO partial pressure by Lander and Germer (#3).
The mean temperature of data collection was 23.6°C.

References
#1. Lux, H. and Ignatowiez, A.
Chem. Ber.(1968) 101,809.
#2. Christensen, A.
J. Cryst. Growth(1976) 33,58.
#3. Lander, J.J. and Germer, L.H.
Trans. Am. Inst. Min. Metall. Pet. Eng.(1948) 175,648.

d(A)	I^{rel}	hkl	2θ(°)
2.608	20	1 0 0	34.355
2.367	25	0 0 2	37.979
2.285	100	1 0 1	39.393
1.7533	20	1 0 2	52.124
1.5059	17	1 1 0	61.529
1.3503	17	1 0 3	69.567
1.3045	2	2 0 0	72.386
1.2705	15	1 1 2	74.647
1.2580	10	2 0 1	75.515
1.1840	3	0 0 4	81.172
1.1423	3	2 0 2	84.804
1.0779	2	1 0 4	91.222
1.0056	3	2 0 3	99.992

Molybdenum Silicide, $MoSi_2$

Synonym
Molybdenum disilicide

Sample
The sample was obtained from Aesar Division of Johnson Matthey, Inc., Seabrook, NH.

Color
Gray

Symmetry classifications

Crystal System	Tetragonal
Space Group	I4/mmm (139)
Pearson Symbol	tI6
Structure Type	C11

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±1

Crystallographic constants of this sample
a = 3.2047 (2) A
c = 7.8449 (8)

c/a = 2.4479

V = 80.57 A^3
Z = 2
Density (calc.) = 6.270 g/cm^3

Figures of merit
F_{18} = 85.9(.0075, 28)
M_{18} = 223.3

Comments
The structure was determined by Zachariasen (#1).
A hexagonal, $CrSi_2$-type is reported to exist below 800°C (#2).
The temperature of data collection was approximately 25.0°C.

Additional patterns
PDF card 6-681
Kieffer and Cerivenka (#3)
Nowotny et al. (#4)

References

#1. Zachariasen, W.H.
Z. Phys. Chem.(1927) 128,39.
#2. Aubry, J. et al.
C. R. Hebd. Seances Acad. Sci.(1965) 261,2665.
#3. Kieffer, R. and Cerivenka, E.
Z. Metallkd.(1952) 43,101.
#4. Nowotny, H. et al.
Monatsh. Chem.(1952) 83,1243.

d(A)	I^{rel}	hkl	2θ(°)
3.923	31	0 0 2	22.647
2.967	60	1 0 1	30.097
2.2661	73	1 1 0	39.745
2.0264	100	1 0 3	44.684
1.9620	23	1 1 2+	46.234
1.6028	21	2 0 0	57.448
1.4832	13	2 0 2+	62.578
1.4098	18	2 1 1	66.241
1.3074	5	0 0 6	72.195
1.2570	33	2 1 3	75.587
1.2411	3	2 0 4	76.730
1.1324	17	1 1 6	85.728
1.0885	2	2 2 2	90.095
1.0584	8	3 0 1	93.399
1.0131	14	2 0 6	98.989
0.9889	6	3 0 3	102.329
0.9813	5	3 1 2+	103.441
0.90025	3	3 1 4	117.663

Niobium Boride, ϵ-NbB_2

Synonym
Niobium diboride

CAS registry no.
12207-29-3

Sample
The sample was obtained from Apache Chemicals, Inc., Seward, IL. It contained a trace of NbB.

Color
Olive gray

Symmetry classifications

Crystal System	Hexagonal
Space Group	P6/mmm (191)
Pearson Symbol	hP3

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Ag
Scanned to	4.0° 2θ
$\sigma(I^{rel})$	±4

Crystallographic constants of this sample
a = 3.11133 (13) A
c = 3.2743 (2)

c/a = 1.0524

V = 27.45 A^3
Z = 1
Density (calc.) = 6.928 g/cm^3

Figures of merit
F_{19} = 120.2(.0079, 20)
M_{19} = 341.1

Comments
The structure was determined by Norton et al. (#1). The temperature of data collection was approximately 25.0°C.

Additional patterns
PDF card 8-120

Reference
#1. Norton, J.T. et al.
Trans. Am. Inst. Min. Metall. Pet. Eng.(1949) 185,749.

d(A)	I^{rel}	hkl	2θ(°)
3.274	33	0 0 1	27.214
2.694	79	1 0 0	33.233
2.0808	100	1 0 1	43.455
1.6366	8	0 0 2	56.155
1.5553	23	1 1 0	59.374
1.4052	20	1 1 1	66.486
1.3994	18	1 0 2	66.796
1.3472	10	2 0 0	69.750
1.2459	17	2 0 1	76.380
1.1279	12	1 1 2	86.148
1.0404	5	2 0 2	95.529
1.0185	5	2 1 0	98.285
1.0117	3	1 0 3	99.174
0.9724	16	2 1 1	104.770
0.89816	3	3 0 0	118.105
0.89341	2	1 1 3	119.129
0.86617	7	3 0 1	125.576
0.86478	10	2 1 2	125.935
0.84804	3	2 0 3	130.552

Potassium Calcium Hydrogen Phosphate, $K_3CaH(PO_4)_2$

Synonym
Potassium calcium hydrogen orthophosphate

Sample
The sample was made by adding 25 ml of a .3 molar solution of calcium acetate to a solution containing 57 grams of K_2HPO_4 and 5 grams of KOH in 72 ml of H_2O.

Color
Colorless

Symmetry classifications

Crystal System	Monoclinic
Space Group	C2/m (12)
Pearson Symbol	mC30

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample

a = 9.8826 (17) A
b = 5.7352 (8)
c = 7.4307 (7)
β = 94.142 (12)°

a/b = 1.7231
c/b = 1.2956

V = 420.07 A^3
Z = 2
Density (calc.) = 2.754 g/cm^3

Figures of merit
F_{30} = 60.5(.0095, 52)
M_{20} = 47.5

Comments
The structure of $K_3Ca(PO_4)_2$ was determined by Grenier et al. (#1).
The mean temperature of data collection was 24.4°C.

Additional patterns
PDF card 22-1218
Majling et al. (#2)

References

#1. Grenier, J.-C., et al. Bull. Soc. Fr. Mineral. Cristallogr.(1969) 92,30.
#2. Majling, J. et al.; (1979) Calculated Powder Diffraction Patterns for Anhydrous Phosphates (VEDA, Bratislava, Czechoslovakia).

d(A)	I^{rel}	hkl	2θ(°)
7.42	9	0 0 1	11.921
4.960	1	1 1 0	17.870
4.249	7	-2 0 1	20.889
4.193	10	-1 1 1	21.170
3.978	1L	2 0 1	22.333
3.707	12	0 0 2	23.989
3.070	33	-2 0 2	29.063
3.021	13	-1 1 2	29.549
2.917	45	1 1 2	30.621
2.867	99	0 2 0+	31.174
2.850	100	3 1 0	31.362
2.470	24	0 0 3	36.336
2.390	5	-4 0 1	37.599
2.375	3	-2 2 1	37.843
2.326	10	2 2 1	38.686
2.289	3	4 0 1	39.338
2.244	1L	-1 1 3	40.161
2.1801	6	1 1 3	41.382
2.1482	1	2 0 3	42.026
2.0949	56	-2 2 2	43.147
2.0258	12	2 2 2	44.697
1.9862	13	4 0 2	45.639
1.9277	1	-3 1 3	47.107
1.8712	3	0 2 3	48.618
1.8526	7	0 0 4	49.139
1.8116	5	3 1 3+	50.326
1.7894	2	4 2 1	50.997
1.7832	1	-2 2 3	51.187
1.7772	1	-2 0 4	51.371
1.7563	1	-1 1 4	52.027
1.7133	9	-5 1 2	53.437
1.6837	2	-1 3 2	54.452
1.6654	7	1 3 2	55.102
1.6523	11	3 3 0	55.574
1.6332	5	4 2 2	56.281
1.5998	3	-3 1 4+	57.567
1.5562	7	0 2 4	59.337
1.5353	3	-4 0 4	60.227
1.5312	1	-4 2 3	60.405
1.5106	5	-2 2 4+	61.318
1.4823	2	0 0 5	62.618
1.4586	3	2 2 4	63.756
1.4487	1	-2 0 5	64.241
1.4344	8	-1 1 5	64.961
1.4254	9	6 2 0	65.422
1.4157	1	-6 0 3	65.926
1.4061	1	1 1 5	66.436
1.3583	2	-2 4 1	69.096
1.3538	1	-4 2 4	69.362
1.3514	1	3 3 3	69.499
1.3499	1	-3 1 5	69.590

Potassium Copper Sulfate Hydrate, $K_2Cu(SO_4)_2 \cdot 6H_2O$

Mineral name
Cyanochroite, syn
Picromerite Group

CAS registry no.
13587-29-6

Sample
The sample was made by evaporation at room temperature of a 1:1 molar aqueous solution of K_2SO_4 and $CuSO_4$.

Color
Brilliant greenish blue

Symmetry classifications

Crystal System	Monoclinic
Space Group	$P2_1/a$ (14)
Pearson Symbol	mP62
Structure Type	A Tutton salt

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	FP Ag
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±3

Crystallographic constants of this sample

a = 9.0800 (14) A
b = 12.123 (2)
c = 6.164 (1)
β = 104.441 (17)°

a/b = 0.7490
c/b = 0.5085

V = 657.08 A^3
Z = 2
Density (calc.) = 2.234 g/cm^3

Figures of merit

F_{30} = 89.0(.0080, 42)
M_{20} = 49.5

Comments
The structure of a Tutton salt, $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$, was determined by Margulis and Templeton (#1).
The mean temperature of data collection was 23.3°C.

References
#1. Margulis, T.N. and Templeton, D.H.
Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.(1962) 117,334.

d(A)	I^{rel}	hkl	2θ(°)
7.120	1L	1 1 0	12.422
6.063	11	0 2 0	14.598
5.971	4	0 0 1	14.825
5.361	11	0 1 1	16.523
5.113	7	-1 1 1	17.329
4.991	5	1 2 0	17.758
4.398	18	2 0 0	20.176
4.254	31	0 2 1	20.867
4.179	90	1 1 1	21.245
4.132	22	2 1 0+	21.488
4.057	79	-2 0 1	21.889
3.848	3	-2 1 1	23.093
3.673	100	1 3 0	24.215
3.589	10	1 2 1	24.785
3.559	11	2 2 0	24.999
3.348	8	0 3 1	26.607
3.281	21	-1 3 1	27.156
3.182	22	2 0 1	28.022
3.075	19	2 1 1	29.015
3.029	18	0 4 0	29.461
2.993	39	1 3 1	29.830
2.975	65	-1 1 2+	30.013
2.899	1L	0 1 2	30.821
2.864	13	1 4 0	31.202
2.849	17	3 1 0	31.378
2.816	42	2 2 1+	31.751
2.738	18	-1 2 2	32.685
2.669	6	-1 4 1	33.544
2.644	13	-3 2 1	33.882
2.555	4	-2 2 2	35.093
2.505	8	1 4 1	35.816
2.497	17	2 4 0	35.936
2.445	2	-1 3 2	36.720
2.3769	45	-3 3 1	37.820
2.3377	2	1 5 0	38.479
2.2533	7	-4 0 1	39.980
2.2463	12	0 5 1	40.109
2.2150	5	-4 1 1	40.701
2.1934	31	2 4 1	41.120
2.1626	1	4 1 0	41.732
2.1264	15	0 4 2	42.478
2.1060	4	3 4 0	42.910
2.0809	7	-2 5 1	43.454
2.0667	28	4 2 0+	43.768
2.0109	3	-2 0 3	45.048
1.9842	15	-2 1 3	45.688
1.9680	2	-4 3 1+	46.084
1.9639	1	0 1 3	46.186
1.9228	5	-4 2 2	47.234
1.9133	4	0 6 1+	47.483
1.8884	5	-3 4 2	48.148
1.8832	6	3 4 1	48.288
1.8676	8	3 5 0	48.717
1.8556	9	-3 1 3	49.053
1.8301	9	-1 3 3	49.782

continued

d(A)	I^{rel}	hkl			2θ(°)
1.8090	7	-2	6	1	50.406
1.8001	6	-2	3	3	50.672
1.7941	7	-3	2	3+	50.852
1.7791	9	4	4	0	51.312
1.7633	1	1	2	3	51.805
1.7411	2	5	1	0	52.518
1.7102	2	-3	5	2	53.540
1.7063	2	2	6	1	53.674
1.6973	2	-5	1	2+	53.981

Potassium Hydrogen Phosphate, KH_2PO_4

Mineral name
Archerite, syn

Synonym
Potassium dihydrogen phosphate
Monobasic potassium phosphate

Sample
The sample was obtained from Allied Chemical Corp., Morristown, NJ.

Color
Colorless

Symmetry classifications

Crystal System	Tetragonal
Space Group	$I\bar{4}2d$ (122)
Pearson Symbol	tI32
Structure Type	Biphosphammite

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample
a = 7.4532 (3) Å
c = 6.9742 (5)

c/a = 0.9357

V = 387.42 A^3
Z = 4
Density (calc.) = 2.333 g/cm^3

Figures of merit
F_{30} = 96.0(.0098, 32)
M_{20} = 110.8

Comments
The structure was determined by West (#1).
An orthorhombic phase is reported by Frazer and Pepinsky (#2) and Ubbelohde and Woodward (#3).
The mean temperature of data collection was 24.3°C.

Additional patterns
PDF card 31-1030, Swanson, H. E. Fuyat, R., and Ugrinic, G. (1954).
Natl. Bur. Stand. (U. S.) Circ. 539, 3, 69.
Hanawalt et al. (#4), Hendricks (#5)

References

#1. West, J.
Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.(1930) 74, 306.
#2. Frazer, B. and Pepinsky, R.
Acta Crystallogr., Sect. A(1953) 6, 273.
#3. Ubbelohde, A. R. and Woodward, I.
Proc. R. Soc. London, Ser. A(1947) A188, 358.
#4. Hanawalt, J. D. et al.
Ind. Eng. Chem., Anal. Ed.(1938) 10, 457.
#5. Hendricks, S. B.
Am. J. Sci.(1927) 14, 269.

d(A)	I^{rel}	hkl	2θ(°)
5.086	14	1 0 1	17.422
3.724	100	2 0 0	23.874
3.008	14	2 1 1	29.674
2.908	83	1 1 2	30.721
2.635	23	2 2 0	33.995
2.547	8	2 0 2	35.214
2.357	5	3 1 0	38.143
2.340	15	3 0 1	38.439
2.218	5	1 0 3	40.636
1.9821	14	3 2 1	45.739
1.9532	51	3 1 2	46.454
1.9064	4	2 1 3	47.664
1.8630	2	4 0 0	48.845
1.7498	1	4 1 1	52.237
1.6981	1	3 0 3	53.954
1.6671	10	4 2 0	55.041
1.5795	8	2 0 4	58.377
1.5686	9	3 3 2	58.821
1.5449	5	3 2 3	59.816
1.5037	1L	4 2 2	61.628
1.4614	2	5 1 0	63.620
1.4579	3	4 3 1	63.791
1.4542	7	2 2 4	63.972
1.4267	1L	4 1 3	65.354
1.4014	1	3 1 4	66.689
1.3707	2	1 0 5	68.385
1.3578	1L	5 2 1	69.128
1.3480	7	5 1 2	69.700
1.3177	3	4 4 0	71.548
1.2868	1	2 1 5	73.544
1.2779	2	5 3 0	74.137
1.2734	9	4 0 4	74.449
1.2546	1	4 3 3	75.756
1.2421	2	6 0 0	76.655
1.2047	6	4 2 4	79.493
1.2002	8	5 3 2	79.855
1.1783	5	6 2 0	81.648
1.1703	1	6 0 2	82.329
1.1562	1L	3 2 5	83.557
1.1349	2	1 1 6	85.485
1.1202	1	5 1 4	86.892
1.0973	1L	6 3 1	89.175
1.0513	1	4 4 4	94.222
1.0425	4	3 1 6	95.275
1.0336	2	6 4 0	96.358
1.0118	4	6 0 4	99.157
1.0090	7	7 1 2	99.536
1.0023	1L	6 3 3	100.449
0.9909	1L	6 4 2	102.045
0.9765	2	6 2 4	104.156
0.9694	1	3 3 6	105.234
0.9422	2	7 3 2	109.680
0.9317	1	8 0 0	111.541
0.90977	2	5 1 6	115.708
0.90382	2	8 2 0	116.918

Potassium Magnesium Phosphate Hydrate, $KMgPO_4 \cdot 6H_2O$

Synonym
Potassium magnesium orthophosphate hydrate

Sample
The sample was prepared by the method of Bassett and Bedwell (#1): 3 grams of $MgCl_2$ in about 50 ml of H_2O were added to a solution of 50 grams of K_2HPO_4 in H_2O. The total volume was diluted to 150 ml. The resultant precipitate crystallized after 3 hours standing at 55°C.

Color
Colorless

Symmetry classifications

Crystal System	Orthorhombic
Space Group	$Pm2_1n$ (31)
Pearson Symbol	oP50
Structure Type	Struvite

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	SI FP
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample

a = 6.8791 (10) A
b = 11.1001 (12)
c = 6.1634 (6)

a/b = 0.6197
c/b = 0.5553

V = 470.63 A^3
Z = 2
Density (calc.) = 1.880 g/cm^3

Figures of merit
F_{30} = 97.7(.0079, 39)
M_{20} = 73.6

Comments
The structure of $KMgPo_4 \cdot 6H_2O$ was determined by Mathew and Schroeder (#2).
The mean temperature of data collection was 24.7°C.

Additional patterns
PDF 20-685

Reference
#1. Bassett, H. and Bedwell, W.L.
J. Chem. Soc.(1933) 877.
#2. Mathew, M. and Schroeder, L.W.
Acta Crystallogr.(1979) B35,11.

d(A)	I^{rel}	hkl	2θ(°)
5.846	10	1 1 0	15.142
5.551	25	0 2 0	15.952
5.390	18	0 1 1	16.434
4.588	17	1 0 1	19.329
4.241	100	1 1 1	20.932
4.123	60	0 2 1	21.538
3.541	6	1 2 1	25.126
3.436	20	2 0 0	25.909
3.258	39	1 3 0	27.353
3.172	6	0 3 1	28.109
3.081	3	0 0 2	28.959
3.004	7	2 0 1	29.718
2.969	18	0 1 2	30.072
2.923	16	2 2 0	30.554
2.899	64	2 1 1	30.814
2.813	7	1 0 2	31.791
2.774	37	0 4 0	32.239
2.726	10	1 1 2	32.834
2.695	55	0 2 2	33.222
2.642	45	2 2 1	33.907
2.531	6	0 4 1	35.437
2.509	8	1 2 2	35.766
2.3743	8	1 4 1	37.862
2.3673	8	0 3 2	37.978
2.3318	12	2 3 1	38.580
2.2946	1	2 0 2	39.230
2.2471	7	2 1 2+	40.094
2.1593	2	2 4 0	41.800
2.1199	5	2 2 2	42.615
2.0540	4	0 0 3	44.051
2.0386	6	2 4 1	44.402
2.0207	1	0 1 3	44.816
1.9987	14	1 5 1	45.338
1.9687	8	1 0 3	46.068
1.9503	18	2 3 2+	46.528
1.9268	7	0 2 3	47.128
1.8561	6	1 2 3	49.040
1.8503	2	0 6 0	49.205
1.8398	4	3 0 2	49.503
1.8151	1L	3 1 2	50.222
1.8007	11	0 5 2	50.652
1.7960	10	0 3 3	50.794
1.7853	8	2 5 1	51.120
1.7640	8	2 0 3	51.784
1.7382	6	1 3 3	52.610
1.7197	9	4 0 0	53.221
1.7165	5	1 6 1	53.329
1.6996	4	3 4 1	53.900
1.6815	2	2 2 3	54.530
1.6473	2	3 3 2	55.760
1.5855	6	0 6 2	58.134
1.5756	5	2 6 1	58.537
1.5449	5	1 7 0+	59.814
1.4990	2	1 7 1	61.844
1.4901	4	1 1 4	62.256

continued

Potassium Magnesium Phosphate Hydrate, $KMgPO_4 \cdot 6H_2O$ (continued)

d(A)	I^{rel}	hkl			2θ(°)
1.4498	3	4	2	2	64.190
1.4222	2	4	4	1+	65.591
1.4136	1L	3	3	3	66.039
1.3930	2	1	3	4	67.145
1.3872	2	0	8	0	67.462
1.3631	2	2	2	4	68.820
1.3485	2	1	6	3	69.674
1.3469	1	0	4	4	69.769

Potassium Nickel Selenate Hydrate, $K_2Ni(SeO_4)_2 \cdot 6H_2O$

Synonym
Dipotassium nickel orthoselenate hexahydrate

Sample
The sample was prepared by dissolving stoichiometric amounts of K_2CO_3, $NiCO_3$, and H_2SeO_4 in water and letting the water evaporate at room temperature.

Color
Unground: strong green
Ground: very pale green

Symmetry classifications

Crystal System	Monoclinic
Space Group	$P2_1/a$ (14)
Pearson Symbol	mP62
Structure Type	A Tutton salt

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	FP Ag
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±5

Crystallographic constants of this sample

a = 9.1760 (9) A
b = 12.3695 (12)
c = 6.2545 (7)
β = 104.404 (9)°

a/b = 0.7418
c/b = 0.5056

V = 687.59 A^3
Z = 2
Density (calc.) = 2.564 g/cm^3

Figures of merit
F_{30} = 90.0(.0083, 40)
M_{20} = 49.3

Comments
The structure of a Tutton salt, $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$, was determined by Margulis and Templeton (#1).
The mean temperature of data collection was 24.0°C.

References
#1. Margulis, T.N. and Templeton, D.H.
Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.(1962) 117,334.

d(A)	I^{rel}	hkl	2θ(°)
7.219	9	1 1 0	12.250
6.188	4	0 2 0	14.301
6.061	1	0 0 1	14.602
5.443	27	0 1 1	16.272
5.079	10	1 2 0	17.445
4.446	22	2 0 0	19.955
4.329	24	0 2 1	20.500
4.236	87	1 1 1	20.956
4.197	63	-1 2 1	21.149
4.106	80	-2 0 1	21.625
3.896	12	-2 1 1	22.809
3.744	100	1 3 0	23.748
3.645	25	1 2 1	24.404
3.612	5	2 2 0	24.629
3.408	21	0 3 1	26.127
3.344	22	-1 3 1	26.636
3.222	27	2 0 1	27.662
3.118	31	2 1 1	28.607
3.093	28	0 4 0	28.844
3.043	31	1 3 1	29.323
3.029	54	0 0 2	29.461
3.019	75	-1 1 2	29.562
2.943	3	0 1 2	30.346
2.908	12	-2 3 1	30.716
2.885	27	-3 1 1	30.967
2.880	27	3 1 0	31.028
2.856	41	2 2 1+	31.293
2.781	16	-2 1 2+	32.155
2.721	4	0 2 2+	32.889
2.672	12	3 2 0	33.516
2.612	3	1 1 2	34.308
2.593	3	-2 2 2	34.570
2.550	8	1 4 1	35.171
2.538	11	2 4 0+	35.337
2.485	8	-1 3 2	36.119
2.468	10	-2 4 1	36.366
2.441	8	0 3 2	36.796
2.411	53	-3 3 1	37.270
2.387	6	3 1 1	37.659
2.3474	3	-2 3 2	38.313
2.2766	3	-4 0 1	39.554
2.2546	3	2 0 2	39.955
2.2325	35	2 4 1	40.369
2.2234	21	4 0 0	40.540
2.1952	3	-1 4 2	41.085
2.1861	11	4 1 0	41.264
2.1637	25	0 4 2	41.711
2.1409	9	-3 4 1	42.177
2.1183	2	-2 5 1+	42.647
2.1008	15	-3 3 2	43.020
2.0958	24	3 3 1	43.128
2.0910	24	4 2 0	43.232
2.0618	2	0 6 0	43.877
2.0515	2	-4 0 2	44.108
2.0197	14	0 0 3	44.841

continued

Potassium Nickel Selenate Hydrate, $K_2Ni(SeO_4)_2 \cdot 6H_2O$ (continued)

d(A)	I^{rel}	hkl			2θ(°)
2.0129	7	-2	1	3	44.999
1.9920	2	0	1	3+	45.499
1.9743	1	-1	2	3	45.929
1.9621	4	2	5	1	46.231
1.9467	3	-4	2	2	46.619
1.9392	6	-1	6	1	46.810
1.9372	5	-1	5	2+	46.860
1.9172	4	-3	4	2+	47.380
1.9129	5	4	1	1+	47.492
1.9003	10	-3	5	1	47.826
1.8814	16	-3	1	3	48.339
1.8740	5	3	1	2+	48.541
1.8614	3	-1	3	3	48.890
1.8426	9	-2	6	1	49.422
1.8370	7	-4	3	2	49.583
1.8329	6	-4	4	1	49.702
1.8279	8	-2	3	3	49.847
1.8224	7	2	4	2	50.008
1.8134	14	-5	1	1+	50.274
1.8046	12	4	4	0	50.535
1.7905	4	1	2	3	50.962
1.7597	11	5	1	0	51.920
1.7381	3	-3	5	2	52.614
1.7329	3	1	7	0	52.784
1.7292	3	-1	4	3+	52.907
1.7187	7	-1	6	2	53.254
1.7157	5	-5	1	2	53.354
1.7084	8	5	2	0	53.603
1.7040	12	1	3	3+	53.751
1.6922	5	3	6	0	54.157
1.6880	2	-1	7	1	54.302
1.6754	2	-4	5	1+	54.745
1.6684	2	-5	2	2	54.995
1.6600	3	-4	2	3	55.296
1.6526	4	4	5	0	55.565
1.6452	6	1	7	1	55.835
1.6410	5	4	4	1	55.993
1.6315	5	1	6	2+	56.346
1.6233	2	-2	7	1	56.657
1.6108	2	4	0	2	57.137
1.5976	7	-5	3	2+	57.652
1.5882	1	5	1	1	58.028
1.5796	2	-4	5	2	58.374
1.5755	2	-3	6	2	58.540
1.5643	2	0	5	3	58.998
1.5563	5	-2	0	4	59.333
1.5491	4	2	7	1	59.639
1.5462	4	0	8	0+	59.759

Potassium Nickel Sulfate Hydrate, $K_2Ni(SO_4)_2 \cdot 6H_2O$

Sample
The sample was made by slow evaporation of a 1:1 molar aqueous solution of K_2SO_4 amd $NiSO_4$.

Color
Strong bluish green

Symmetry classifications

Crystal System	Monoclinic
Space Group	$P2_1/a$ (14)
Pearson Symbol	mP62
Structure Type	A Tutton salt

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	Ag FP
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±3

Crystallographic constants of this sample

a = 8.9984 (12) A
b = 12.182 (2)
c = 6.1321 (8)
β = 105.054 (13)°

a/b = 0.7387
c/b = 0.5034

V = 649.12 A^3
Z = 2
Density (calc.) = 2.236 g/cm^3

Figures of merit
F_{30} = 85.1(.0084, 42)
M_{20} = 52.3

Comments
The structure of a Tutton salt $(NH_4)_2Mg(SO_4)_2 \cdot 6H_2O$, was determined by Margulis and Templeton (#1).
The mean temperature of data collection was 24.1°C.

Additional patterns
PDF card 13-193

References
#1. Margulis, T.N. and Templeton, D.H.
Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.(1962) 117,334.

d(A)	I^{rel}	hkl	2θ(°)
6.095	9	0 2 0	14.522
5.924	3	0 0 1	14.943
5.327	10	0 1 1	16.628
5.105	6	-1 1 1	17.356
4.344	22	2 0 0	20.426
4.245	23	0 2 1	20.909
4.131	86	1 1 1+	21.493
4.092	29	2 1 0	21.701
4.037	85	-2 0 1	22.000
3.834	5	-2 1 1	23.179
3.678	100	1 3 0	24.177
3.563	9	1 2 1	24.973
3.536	7	2 2 0	25.162
3.350	10	0 3 1	26.589
3.292	18	-1 3 1	27.068
3.137	17	2 0 1	28.433
3.038	36	2 1 1	29.374
2.962	62	0 0 2+	30.152
2.879	4	0 1 2	31.034
2.875	4	1 4 0	31.080
2.866	4	-2 3 1	31.177
2.839	9	-3 1 1	31.485
2.820	21	3 1 0	31.705
2.810	21	-2 0 2	31.821
2.789	22	2 2 1	32.070
2.739	19	-2 1 2	32.668
2.731	19	-1 2 2	32.771
2.678	6	-1 4 1	33.439
2.632	5	-3 2 1	34.030
2.550	3	-2 2 2	35.161
2.495	7	2 4 0	35.961
2.481	8	2 3 1	36.177
2.442	1	-1 3 2	36.778
2.393	6	1 2 2+	37.549
2.369	44	-3 3 1	37.953
2.2528	6	0 5 1	39.988
2.2362	5	-4 0 1+	40.298
2.1993	11	-4 1 1	41.005
2.1861	25	2 4 1	41.263
2.1718	10	4 0 0	41.549
2.1611	1L	2 1 2	41.763
2.1386	4	4 1 0	42.223
2.1304	8	1 5 1	42.394
2.1232	13	0 4 2	42.545
2.1070	5	-3 4 1	42.888
2.0992	5	-4 2 1+	43.056
2.0859	6	-2 5 1	43.344
2.0651	11	-2 4 2+	43.803
2.0459	13	4 2 0	44.235
2.0185	1	-4 0 2	44.869
2.0042	3	-2 0 3	45.206
1.9734	15	0 0 3	45.951
1.9587	1	-4 3 1	46.316
1.9369	1L	-1 2 3	46.868
1.9241	4	2 5 1	47.200

continued

Potassium Nickel Sulfate Hydrate, $K_2Ni(SO_4)_2 \cdot 6H_2O$ (continued)

d(A)	I^{rel}	hkl			2θ(°)
1.9151	2	4	3	0	47.434
1.9106	6	-1	6	1	47.552
1.8876	6	4	0	1+	48.170
1.8707	6	3	4	1+	48.631
1.8660	7	4	1	1	48.764
1.8516	2	-3	1	3	49.167
1.8386	5	2	6	0	49.539
1.8246	1	-1	3	3+	49.945
1.8085	3	-4	3	2	50.419
1.8044	7	1	1	3	50.541
1.7970	4	-2	3	3	50.764
1.7809	6	2	4	2	51.256

Potassium Phosphate, KPO_3

Synonym
Potassium metaphosphate
Potassium polyphosphate

Sample
The sample was made by heating KH_2PO_4 overnight at about 300°C.

Color
Colorless

Symmetry classifications

Crystal System	Monoclinic
Space Group	$P2_1/a$ (14)
Pearson Symbol	mP40

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Ag
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±4

Crystallographic constants of this sample

a = 14.067 (2) A
b = 4.5464 (13)
c = 10.3272 (19)
β = 101.093 (16)°

a/b = 3.0941
c/b = 2.2715

V = 648.13 A^3
Z = 8
Density (calc.) = 2.420 g/cm^3

Figures of merit
F_{30} = 61.8(.0077, 63)
M_{20} = 49.7

Comments
The structure of KPO_3 was determined by Jost (#1). There are several other forms of KPO_3 stable at higher temperatures (#2).
The mean temperature of data collection was 24.3°C.

Additional patterns
PDF card 25-669

References

#1. Jost, K.H.
Acta Crystallogr.(1963) 16,623.
#2. Jost, K.H., and Schulze, H.J.
Acta Crystallogr., Sect. B(1969) B25,1110.

d(A)	I^{rel}	hkl	2θ(°)
10.15	1	0 0 1	8.704
6.298	39	-2 0 1	14.050
5.249	15	2 0 1	16.878
5.065	27	0 0 2	17.494
4.517	13	-2 0 2	19.639
3.754	17	2 0 2	23.681
3.687	7	-2 1 1	24.121
3.451	73	4 0 0	25.797
3.438	71	2 1 1	25.894
3.384	100	0 1 2+	26.316
3.295	19	-2 0 3	27.040
3.234	3	3 1 0	27.560
3.147	24	-4 0 2	28.338
3.090	13	4 0 1	28.869
2.909	1	-3 1 2	30.710
2.828	16	2 0 3	31.615
2.762	27	-4 1 1	32.384
2.749	28	4 1 0	32.550
2.685	20	-4 0 3	33.347
2.668	14	-2 1 3	33.565
2.588	15	-4 1 2+	34.631
2.513	1L	-3 1 3	35.700
2.4001	4	2 1 3	37.440
2.3866	3	-5 1 1	37.660
2.3009	7	6 0 0	39.119
2.2750	60	4 1 2+	39.583
2.2660	31	-6 0 2	39.746
2.2456	6	-1 1 4	40.122
2.2200	30	5 1 1	40.606
2.2140	22	0 1 4	40.720
2.0995	1	-6 0 3	43.049
2.0532	6	6 1 0+	44.070
2.0270	6	0 0 5+	44.669
1.9574	2	6 0 2	46.350
1.9490	3	-3 2 2+	46.560
1.8976	6	4 2 0	47.899
1.8939	5	-6 0 4	47.999
1.8786	7	-1 1 5	48.415
1.8718	8	-2 1 5+	48.602
1.8521	5	0 1 5	49.152
1.8432	7	-4 2 2	49.407
1.7995	5	5 1 3	50.690
1.7935	6	1 1 5	50.870
1.7721	4	2 2 3	51.530
1.7585	1	-8 0 1	51.959
1.7484	3	-6 1 4	52.282
1.7350	6	4 1 4+	52.714

Potassium Sodium Phosphate, $KNa_2(PO_3)_3$

Synonym
Potassium disodium metaphosphate

Sample
The sample was made by heating a 1:2 molar mixture of KH_2PO_4 and NaH_2PO_4 at 500°C for 3 hours.

Color
Colorless

Symmetry classifications

Crystal System	Triclinic
Space Group	$P\bar{1}$ (2)
Pearson Symbol	aP30

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	Si FP
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample

a = 6.8696 (15) A
b = 9.4671 (17)
c = 6.7886 (15)
α = 110.086 (13)°
β = 104.659 (16)
γ = 86.581 (15)

a/b = 0.7256
c/b = 0.7171

V = 400.97 A^3
Z = 2
Density (calc.) = 2.667 g/cm^3

Figures of merit
F_{30} = 57.9(.0084, 62)
M_{20} = 39.4

Comments
The structure of $KNa_2(PO_3)_3$ was determined by Tordjman et al. (#1).
The temperature of data collection was approximately 25.0°C.

Additional patterns
PDF card 26-969
Majling et al. (#2)

References

#1. Tordjman, I. et al.
Acta Crystallogr., Sect. B(1974) B30,2701.
#2. Majling, J. et al.; (1979)
Calculated Powder Diffraction Patterns for Anhydrous Phosphates (VEDA, Bratislava, Czechoslovakia).

d(A)	I^{rel}	hkl	2θ(°)
8.90	15	0 1 0	9.934
6.178	7	0 0 1	14.325
5.401	7	-1 1 0	16.400
5.249	13	1 1 0	16.876
5.126	34	-1 -1 1	17.284
4.444	20	0 2 0	19.964
4.383	4	0 -2 1	20.245
4.054	7	-1 1 1+	21.904
3.434	3	1 -2 1	25.928
3.390	2	1 1 1	26.266
3.287	13	-2 0 1+	27.110
3.243	4	-2 -1 1	27.479
3.141	27	-2 1 0	28.394
3.110	33	-1 0 2	28.680
3.089	22	0 0 2	28.880
3.063	13	-1 -2 2	29.126
3.014	14	-1 2 1	29.617
2.962	100	0 3 0	30.148
2.856	9	-2 -2 1	31.300
2.724	14	1 -3 1	32.847
2.701	31	-2 -1 2+	33.137
2.689	24	1 2 1	33.290
2.680	20	2 -1 1	33.406
2.673	13	-1 1 2+	33.498
2.624	16	2 2 0	34.139
2.576	5	1 -2 2	34.798
2.568	6	1 0 2	34.914
2.478	1L	2 -2 1	36.220
2.438	8	2 1 1	36.830
2.3417	2	-2 1 2	38.410
2.3257	1	-1 3 1	38.684
2.3044	3	1 3 2	39.057
2.2776	3	-2 -3 2	39.536
2.2715	5	-1 -4 1+	39.645
2.2438	3	-2 3 0+	40.157
2.2279	4	-1 2 2	40.456
2.2215	4	0 4 0	40.577
2.2091	1	0 2 2	40.815
2.1747	4	0 -1 3+	41.491
2.1289	1	2 2 1	42.425
2.0866	7	2 -1 2	43.329
2.0514	4	-2 3 1	44.110
2.0283	4	-2 2 2+	44.640
1.9957	4	1 -4 2	45.410
1.9589	1	3 2 0	46.310
1.9215	1	-3 1 2+	47.268
1.8954	5	0 4 1	47.959
1.8780	7	2 1 2	48.431
1.8738	5	-1 4 1+	48.548
1.8467	5	0 3 2	49.307
1.8420	3	1 0 3+	49.444
1.8218	3	2 4 0+	50.025

Potassium Titanium Oxide Phosphate, $KTiOPO_4$

Sample
The sample was prepared by heating a 1:2:2 molar mixture of K_2CO_3, TiO_2 (anatase), and $NH_4H_2PO_4$ up to 500°C. It was then reground and heated at 1000°C overnight.

Color
Colorless

Symmetry classifications

Crystal System	Orthorhombic
Space Group	$P2_1nb$ (33)
Pearson Symbol	oP64

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±4

Crystallographic constants of this sample

a = 10.5892 (12) A
b = 12.8149 (11)
c = 6.4032 (5)

a/b = 0.8263
c/b = 0.4997

V = 868.93 A^3
Z = 8
Density (calc.) = 3.027 g/cm^3

Figures of merit
F_{30} = 114.9(.0061, 43)
M_{20} = 70.0

Comments
The structure was determined by Tordjman et al. (#1). The mean temperature of data collection was 24.7°C.

Additional patterns
PDF card 25-689

Reference
#1. Tordjman, I. et al.
Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.(1974) 139,103.

d(A)	I^{rel}	hkl	2θ(°)
6.404	10	0 2 0	13.818
5.724	18	0 1 1	15.468
5.477	79	1 0 1+	16.169
5.039	1	1 1 1	17.587
4.535	1L	0 2 1	19.558
4.166	10	1 2 1	21.310
4.083	1	2 2 0	21.747
3.887	1L	2 1 1	22.860
3.554	9	0 3 1	25.037
3.442	31	2 2 1	25.864
3.368	20	1 3 1	26.440
3.091	79	3 0 1+	28.859
3.005	5	3 1 1	29.710
2.980	8	1 1 2	29.960
2.951	2	2 3 1	30.260
2.864	5	0 2 2+	31.203
2.766	100	1 4 1+	32.344
2.741	72	2 4 0+	32.647
2.6786	4	2 1 2	33.426
2.6472	12	4 0 0	33.834
2.5604	1	0 3 2	35.018
2.5195	10	2 4 1+	35.604
2.5040	3	3 3 1	35.832
2.4899	1	1 3 2	36.042
2.4468	1L	4 2 0	36.700
2.4031	4	4 1 1	37.391
2.3794	5	0 5 1	37.779
2.3312	3	3 1 2	38.590
2.3209	1	1 5 1	38.768
2.3065	1L	2 3 2	39.020
2.2641	7	0 4 2	39.780
2.2237	6	3 2 2+	40.536
2.1700	10	2 5 1	41.585
2.1362	3	0 6 0	42.273
2.1225	1L	4 3 1	42.560
2.1053	11	0 1 3	42.924
2.0927	1	1 0 3+	43.196
2.0733	3	3 3 2	43.621
2.0401	30	4 0 2+	44.368
2.0103	6	5 0 1+	45.060
1.9902	4	1 6 1+	45.541
1.9804	1	2 6 0	45.780
1.9662	3	1 5 2	46.130
1.9565	4	2 1 3	46.372
1.9441	1	4 2 2+	46.685
1.9095	4	0 3 3	47.581
1.8918	5	2 2 3+	48.056
1.8792	2	1 3 3	48.399
1.8272	14	3 6 0+	49.868
1.8080	1L	3 1 3	50.434
1.7954	1L	2 3 3	50.812
1.7770	5	0 6 2+	51.378
1.7696	6	4 5 1	51.608
1.7568	9	3 2 3+	52.013
1.7519	6	1 4 3+	52.167
1.7407	3	3 5 2	52.531
1.7364	1	1 7 1	52.671
1.7207	19	4 4 2	53.188
1.7028	13	5 2 2+	53.791
1.6868	2	6 1 1	54.344
1.6796	4	3 3 3	54.596
1.6477	5	4 1 3	55.746
1.6208	1	1 5 3	56.753
1.6019	17	0 8 0	57.483
1.5868	4	3 4 3+	58.083

continued

d(A)	I^{rel}	hkl	2θ(°)
1.5754	2	3 7 1	58.542
1.5715	3	1 7 2+	58.705
1.5670	3	2 5 3	58.890
1.5532	3	0 2 4	59.462
1.5489	6	4 3 3	59.644
1.5459	10	6 4 0+	59.773
1.5371	2	1 8 1+	60.152
1.5331	1	2 8 0	60.322
1.5218	1	2 7 2+	60.817

Potassium Zirconium Phosphate, $KZr_2(PO_4)_3$

Synonym
Potassium zirconium orthophosphate

CAS registry no.
19527-82-3

Sample
The sample was made by heating a 1:2:3 molar mixture of KH_2PO_4, ZrO_2, and $NH_4H_2PO_4$ up to 1150°C for 2 hrs.

Color
Colorless

Symmetry classifications

Crystal System	Rhombohedral
Space Group	$R\bar{3}c$ (167)
Pearson Symbol	hR36

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	Si FP
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample
(Hexagonal axes)
a = 8.7191 (3) A
c = 23.9445 (12)

c/a = 2.7462

V = 1576.45 A^3
Z = 6
Density (calc.) = 3.201 g/cm^3

Figures of merit
F_{30} = 133.5(.0058, 39)
M_{20} = 101.4

Comments
The structure of $KZr_2(PO_4)_3$ was determined by Sljukic et al. (#1).
The mean temperature of data collection was 23.7°C.

Additional patterns
PDF card 25-1206
Majling et al. (#2)

References

#1. Sljukic, M. et al.
Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.(1969) 130,148.
#2. Majling, J. et al.; (1979)
Calculated Powder Diffraction Patterns for Anhydrous Phosphates (VEDA, Bratislava, Czechoslovakia).

d(A)	I^{rel}	hkl	2θ(°)
6.393	11	0 1 2	13.840
4.695	26	1 0 4	18.887
4.363	65	1 1 0	20.338
3.828	61	1 1 3	23.220
3.194	37	0 2 4	27.909
2.944	100	1 1 6	30.331
2.835	8	2 1 1	31.534
2.7833	6	0 1 8	32.134
2.5761	8	2 1 4	34.797
2.5173	33	3 0 0	35.637
2.4518	1	1 2 5	36.622
2.3454	5	2 0 8	38.347
2.2828	3	1 0 10	39.441
2.2714	7	1 1 9	39.647
2.1916	2	2 1 7	41.156
2.1799	5	2 2 0	41.387
2.1291	16	3 0 6	42.421
2.1031	2	2 2 3	42.972
2.0866	1	1 3 1	43.329
2.0655	11	1 2 8	43.793
2.0221	8	0 2 10	44.783
1.9953	3	0 0 12	45.420
1.9769	8	1 3 4	45.866
1.9129	30	2 2 6	47.493
1.8645	3	0 4 2	48.805
1.8343	19	2 1 10	49.663
1.8143	1	1 1 12	50.248
1.7860	4	1 3 7	51.100
1.7157	5	3 1 8	53.354
1.6860	1	2 2 9	54.371
1.6681	4	0 1 14	55.003
1.6640	8	3 2 4	55.152
1.6478	19	4 1 0	55.742
1.6289	1	2 3 5	56.444
1.6137	2	4 1 3	57.025
1.5965	3	0 4 8	57.697
1.5763	10	1 3 10	58.507
1.5637	7	3 0 12	59.025
1.5578	9	2 0 14	59.270
1.5474	1	2 1 13	59.709
1.5230	12	4 1 6	60.765
1.5093	1	3 1 11	61.376
1.4990	1	1 1 15	61.846
1.4824	3	4 0 10	62.613
1.4673	1	1 2 14	63.332
1.4641	9	0 5 4	63.488
1.4533	5	3 3 0	64.016
1.4298	1	3 3 3	65.194
1.4034	2	3 2 10	66.578
1.3914	1	0 2 16	67.232
1.3882	1	2 4 4	67.404
1.3655	2	3 3 6	68.683
1.3541	1	5 1 1	69.339
1.3302	1	0 0 18	70.775
1.3248	7	3 1 14	71.103

continued

d(A)	I^{rel}	hkl	2θ(°)
1.3225	8	5 1 4	71.249
1.3048	1L	1 5 5	72.366
1.2706	1	4 1 12	74.639
1.2673	1	0 4 14	74.865
1.2629	2	1 2 17	75.173
1.2606	4	5 1 7	75.335
1.2585	2	6 0 0	75.483

Silver Titanium Phosphate, $AgTi_2(PO_4)_3$

Synonym
Silver titanium orthophosphate

CAS registry no.
30622-40-3

Sample
The sample was made by heating a 1:2:3 molar mixture of $AgNO_3$, TiO_2 (anatase), and $(NH_4)_2HPO_4$ at 750° C overnight and at 1100°C for 40 hours.

Color
Colorless

Symmetry classifications

Crystal System	Rhombohedral
Space Group	$R\bar{3}c$ (167)
Pearson Symbol	hR36

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	4.0° 2θ
$\sigma(I^{rel})$	±5

Crystallographic constants of this sample
(Hexagonal axes)
a = 8.4734 (5) A
c = 22.114 (2)

c/a = 2.6098

V = 1375.03 A^3
Z = 6
Density (calc.) = 3.540 g/cm^3

Figures of merit
F_{30} = 71.5(.0100, 42)
M_{20} = 62.2

Comments
Isostructural with other titanium or zirconium double phosphates with alkalis (#1).
The temperature of data collection was approximately 25.0°C.

Additional patterns
PDF card 25-768

Reference
#1. Masse, R.
Bull. Soc. Fr. Mineral. Cristallogr.(1970) 93,500.

d(A)	I^{rel}	hkl	2θ(°)
6.109	8	0 1 2	14.488
4.412	1	1 0 4	20.112
4.236	60	1 1 0	20.956
3.670	62	1 1 3	24.235
3.481	36	2 0 2	25.572
3.058	2	0 2 4	29.184
2.782	100	1 1 6	32.147
2.753	10	2 1 1	32.496
2.691	18	1 2 2	33.268
2.589	9	0 1 8	34.625
2.479	5	2 1 4	36.202
2.447	33	3 0 0	36.699
2.208	10	2 0 8	40.844
2.1254	16	1 1 9	42.498
2.1175	13	1 0 0+	42.665
2.0845	2	2 1 7	43.374
2.0385	13	3 0 6	44.404
2.0023	2	3 1 2	45.252
1.9580	22	1 2 8	46.334
1.8434	2	0 0 12	49.399
1.8365	27	2 2 6	49.599
1.7406	3	4 0 4	52.534
1.7287	1	2 1 10	52.922
1.7110	3	1 3 7	53.515
1.6897	2	1 1 12	54.243
1.6639	3	2 3 2	55.156
1.6387	8	3 1 8	56.078
1.6103	1	3 2 4	57.156
1.6014	22	4 1 0	57.505
1.5732	1	2 3 5	58.634
1.5648	2	4 1 3	58.981
1.5438	2	0 1 14	59.861
1.5285	5	0 4 8	60.522
1.4978	1	1 3 10	61.898
1.4859	1	3 2 7	62.453
1.4720	11	3 0 12	63.106
1.4689	12	4 1 6	63.258
1.4509	6	2 0 14	64.132
1.4378	2	2 3 8	64.790
1.4302	2	3 1 11	65.174
1.4187	1	0 5 4	65.773
1.4124	2	3 3 0+	66.101
1.3920	2	1 1 15	67.198
1.3868	2	3 3 3	67.486
1.3761	1L	4 2 2	68.077
1.3725	5	1 2 14	68.281
1.3416	1	4 1 9	70.080
1.3187	1	3 3 6	71.487
1.3049	1L	1 3 13	72.355
1.2908	1L	2 3 11	73.276
1.2630	1	1 5 5	75.163
1.2479	4	3 1 14	76.232
1.2229	3	0 5 10+	78.085

Sodium Germanium Fluoride, Na_2GeF_6

Synonym
Sodium hexafluorogermanate

CAS registry no.
21087-90-1

Sample
The sample was obtained from STREM Chemicals, Inc. Newburyport, MA.

Color
Colorless

Symmetry classifications

Crystal System	Hexagonal
Space Group	P321 (150)
Pearson Symbol	hP27
Structure Type	Na_2SiF_6

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	W
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample
a = 9.0583 (2) A
c = 5.1088 (2)

c/a = 0.5640

V = 363.03 A^3
Z = 3
Density (calc.) = 3.191 g/cm^3

Figures of merit
F_{30} = 126.4(.0058, 41)
M_{20} = 114.6

Comments
The structure was originally determined by Cipriani (#1). Zalkin et al. (#2) found that the earlier space group was incorrect.
The mean temperature of data collection was 24.9°C.

Additional patterns
Cox (#3)

References

#1. Cipriani, C.
Rend. Soc. Mineral. Ital.(1955) 11,58.
#2. Zalkin, A. et al.
Acta Crystallogr.(1964) 17,1408.
#3. Cox, B.
J. Chem. Soc.(1954) 3251.

d(A)	I^{rel}	hkl	2θ(°)
5.112	9	0 0 1	17.334
4.530	100	1 1 0	19.580
4.283	87	1 0 1	20.722
3.390	35	1 1 1	26.267
3.111	45	2 0 1	28.669
2.964	3	2 1 0	30.127
2.6144	13	3 0 0	34.271
2.5644	26	2 1 1	34.961
2.3276	37	3 0 1	38.652
2.2637	1	2 2 0	39.789
2.2239	4	1 1 2	40.532
2.1757	1	3 1 0	41.471
2.1402	2	2 0 2	42.191
2.0702	3	2 2 1	43.690
2.0019	4	3 1 1	45.261
1.9354	3	2 1 2	46.907
1.8273	45	3 0 2	49.865
1.7997	1	3 2 0	50.683
1.7118	7	4 1 0	53.488
1.6942	25	2 2 2	54.089
1.6562	2	3 1 2	55.432
1.6231	8	4 1 1	56.666
1.5940	2	1 1 3	57.797
1.5622	4	2 0 3	59.087
1.5556	1	4 0 2	59.361
1.5097	12	3 3 0	61.360
1.5000	5	5 0 1	61.801
1.4826	5	4 2 0	62.603
1.4767	8	2 1 3	62.885
1.4481	1L	3 3 1	64.273
1.4271	13	3 0 3	65.336
1.4220	4	4 1 2	65.598
1.3609	4	2 2 3	68.945
1.3580	3	5 1 1	69.115
1.3410	4	3 1 3	70.120
1.3075	3	6 0 0	72.189
1.2996	1L	3 3 2	72.699
1.2858	1L	4 0 3	73.608
1.2773	1L	0 0 4	74.183
1.2665	1L	6 0 1	74.919
1.2562	4	5 2 0	75.646
1.2504	1	4 3 1	76.055
1.2368	3	3 2 3	77.043
1.2338	1	5 1 2	77.268
1.2291	1	1 1 4	77.615
1.2199	1L	5 2 1	78.314
1.2071	1	4 1 3	79.310
1.1732	1L	2 1 4	82.083
1.1637	3	6 0 2	82.894
1.1538	1L	5 0 3	83.765
1.1477	1	3 0 4	84.318
1.1323	1	4 4 0	85.732
1.1273	1L	5 2 2	86.204
1.1183	1L	4 2 3	87.074
1.1124	1L	2 2 4	87.652

continued

d(A)	I^{rel}	hkl			2θ(°)
1.1055	1L	4	4	1	88.339
1.1014	1L	3	1	4	88.758
1.0948	1	5	3	1	89.433
1.0855	1	5	1	3	90.408
1.0834	1L	6	1	2	90.637
1.0701	1L	4	0	4	92.082
1.0641	1	6	2	1	92.759
1.04171	1L	3	2	4	95.370
1.03912	1L	7	1	0	95.684
1.03509	1L	4	4	2	96.178
1.02815	1L	4	3	3	97.044
1.02627	1	5	3	2	97.282
1.02375	1L	4	1	4	97.602
1.01836	1L	7	1	1	98.298
1.01328	1	1	0	5	98.964
1.01078	1L	5	2	3	99.296
0.99685	1L	1	1	5	101.200
0.98847	1	6	3	0	102.390
0.98550	1	5	4	1	102.821
0.97897	1L	6	1	3	103.784
0.97501	1	3	3	4	104.379
0.97038	1L	6	3	1	105.086
0.96603	1L	2	1	5	105.762
0.96243	2	7	1	2	106.331
0.94205	1	7	2	1	109.708
0.93608	1L	5	3	3	110.753
0.92168	1	6	3	2	113.390
0.91673	1L	6	2	3	114.337
0.91366	1	6	0	4	114.935
0.90589	1L	5	5	0	116.494
0.90362	1L	8	1	1	116.961

Sodium Magnesium Hydrogen Phosphate, $Na_3MgH(PO_4)_2$

Synonym
Sodium magnesium hydrogen orthophosphate

Sample
The sample was prepared by the method of Bassett and Bedwell (#1): 3 grams of $MgCl_2$ in about 50 ml of H_2O were added to a solution of 39.64 grams of Na_2HPO_4 in H_2O. The total volume was diluted to 150 ml. The resultant precipitate slowly crystallized after standing in a stoppered flask at 55°C for 3 days.

Color
Colorless

Symmetry classifications

Crystal System	Triclinic
Space Group	P1 (1)
Pearson Symbol	aP15

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample

a = 5.2305 (9) A
b = 6.8224 (8)
c = 5.1774 (7)
α = 91.563 (11)°
β = 117.502 (12)
γ = 90.439 (12)

a/b = 0.7667
c/b = 0.7589

V = 163.77 A^3
Z = 1
Density (calc.) = 2.882 g/cm^3

Figures of merit
F_{30} = 60.6(.0105, 47)
M_{20} = 51.4

Comments
The cell was obtained by the use of Visser's program.
The mean temperature of data collection was 24.3°C.

Additional patterns
PDF card 15-124

Reference
#1. Bassett, H. and Bedwell, W.L.
J. Chem. Soc.(1933) 877.

d(A)	I^{rel}	hkl	2θ(°)
6.80	13	0 1 0	13.001
4.643	3	1 0 0	19.098
4.451	3	-1 0 1	19.931
3.875	37	-1 1 0+	22.934
3.795	14	1 1 0	23.421
3.746	48	-1 -1 1	23.733
3.707	16	-1 1 1	23.989
3.410	36	0 2 0	26.110
2.783	55	0 -2 1	32.134
2.718	50	1 2 0	32.931
2.697	100	1 0 1	33.196
2.612	50	-2 0 1	34.299
2.587	47	-1 0 2	34.651
2.538	3	1 -1 1	35.343
2.481	1L	1 1 1	36.170
2.435	4	-2 -1 1	36.889
2.318	18	2 0 0	38.812
2.295	19	0 0 2	39.229
2.273	24	0 3 0	39.616
2.223	3	-2 0 2	40.539
2.199	2	0 -1 2	41.007
2.182	2	2 1 0	41.350
2.153	3	0 1 2+	41.931
2.1221	7	-2 -1 2	42.567
2.1064	7	-2 1 2	42.900
2.0864	4	-1 -2 2	43.333
2.0802	3	-2 2 1	43.469
2.0594	4	-1 3 0	43.930
2.0340	3	-1 -3 1+	44.509
2.0145	15	-1 3 1	44.963
2.0092	9	0 3 1	45.087
1.9381	28	-2 2 0	46.839
1.8975	4	2 2 0	47.903
1.8733	45	-2 -2 2+	48.561
1.8533	1	-2 2 2	49.120
1.7678	1	1 -3 1	51.665
1.7587	1L	1 0 2	51.953
1.7192	8	-2 3 1	53.238
1.7044	18	0 4 0	53.736
1.6855	6	-1 3 2	54.389
1.6674	1L	-1 -1 3	55.030
1.6424	8	-2 3 0+	55.940
1.6264	1L	-2 1 3	56.540
1.6122	1L	-1 4 0	57.084
1.6049	2	2 3 0	57.366
1.5995	2	-2 -3 2	57.580
1.5864	8	1 -2 2+	58.097
1.5452	20	-1 -2 3	59.801
1.5408	11	1 2 2	59.989
1.5307	12	0 0 3	60.430
1.5222	4	-2 -2 3	60.802
1.5177	1	-3 2 2	60.999
1.5073	6	-1 2 3	61.469
1.4967	3	-2 2 3	61.950
1.4822	3	0 1 3+	62.623

continued

d(A)	I^{rel}	hkl	2θ(°)
1.4633	2	1 -4 1	63.525
1.4404	8	-1 -4 2	64.660
1.4315	6	-2 4 1	65.108
1.4232	10	-2 -4 1	65.535
1.4195	7	1 4 1	65.729
1.4066	5	-1 4 2	66.411

Sodium Rhenium Oxide, $NaReO_4$

Synonym
Sodium perrhenate

CAS registry no.
13472-33-8

Sample
The sample was obtained from STREM Chemical, Inc., Newburyport, MA.

Color
Colorless

Symmetry classifications

Crystal System	Tetragonal
Space Group	$I4_1/a$ (88)
Pearson Symbol	tI24
Structure Type	$CaWO_4$

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	W
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample

a = 5.37330 (16) A
c = 11.7428 (5)

c/a = 2.1854

V = 339.04 A^3
Z = 4
Density (calc.) = 5.352 g/cm^3

Figures of merit
F_{30} = 131.4(.0067, 34)
M_{20} = 152.6

Comments
The structure was determined by Beintema (#1).
The temperature of data collection was approximately 25.0°C.

Reference
#1. Beintema, J.
Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.(1937) 97,300.

d(A)	I^{rel}	hkl	2θ(°)
4.884	81	1 0 1	18.149
3.188	100	1 1 2	27.963
3.163	36	1 0 3	28.190
2.935	13	0 0 4	30.431
2.686	15	2 0 0	33.329
2.4441	1	2 0 2	36.742
2.3541	23	2 1 1	38.199
2.3235	2	1 1 4	38.723
2.1523	6	1 0 5	41.942
2.0469	12	2 1 3	44.213
1.9818	25	2 0 4	45.745
1.8997	10	2 2 0	47.843
1.7705	4	3 0 1	51.581
1.7400	10	1 1 6	52.553
1.6797	11	2 1 5	54.591
1.6325	24	3 1 2	56.309
1.6285	15	3 0 3	56.459
1.6015	8	1 0 7	57.501
1.5950	12	2 2 4	57.758
1.4783	5	3 2 1	62.806
1.4678	2	0 0 8	63.307
1.4243	3	3 0 5	65.480
1.3926	4	3 2 3	67.166
1.3753	5	2 1 7	68.123
1.3691	1L	1 1 8	68.478
1.3434	2	4 0 0	69.973
1.3096	1L	4 0 2	72.057
1.2953	3	4 1 1	72.982
1.2880	5	2 0 8	73.460
1.2831	8	3 1 6	73.789
1.2680	1	1 0 9	74.815
1.2582	2	3 2 5	75.502
1.2381	6	3 3 2	76.947
1.2364	3	4 1 3	77.074
1.2245	5	3 0 7	77.965
1.2218	9	4 0 4	78.169
1.2017	3	4 2 0	79.735
1.1771	1L	4 2 2	81.747
1.1617	2	2 2 8	83.071
1.1467	2	2 1 9	84.403
1.1395	1	4 1 5	85.065
1.1220	2	1 1 10	86.715
1.1142	2	3 2 7	87.477
1.1119	4	4 2 4	87.702
1.0702	2	4 3 1	92.067
1.0634	2	3 3 6	92.836
1.0546	1	3 0 9	93.848
1.0470	1	1 0 11	94.736
1.0372	6	5 1 2	95.917
1.0363	2	4 3 3	96.031
1.0290	1	4 1 7	96.936
0.99413	1	5 2 1	101.583
0.99098	1	4 0 8	102.030
0.98172	1L	3 2 9	103.375
0.97856	1	0 0 12	103.845

Strontium Chromium Oxide, $SrCrO_4$

Synonym
Strontium chromate

CAS registry no.
7789-06-2

Sample
A sample of strontium chromate was heated at 500°C for 2 days.

Color
Brilliant yellow

Symmetry classifications
Crystal System Monoclinic
Space Group $P2_1/n$ (14)
Pearson Symbol mP24

Data collection and analysis parameters
Radiation $CuK\alpha_1$
Wavelength 1.5405981 A
2θ Standard Si
Scanned to 4.0° 2θ
$\sigma(I^{rel})$ ±2

Crystallographic constants of this sample
a = 7.0897 (4) A
b = 7.3939 (4)
c = 6.7553 (6)
β = 103.197 (5)°

a/b = 0.9589
c/b = 0.9136

V = 344.76 A^3
Z = 4
Density (calc.) = 3.923 g/cm^3

Figures of merit
F_{30} = 113.2(.0049, 54)
M_{20} = 87.5

Comments
The structure was determined by Pistorius and Pistorius (#1).
Pistorius and Pistorius (#1) suggest a second form of $SrCrO_4$ which is orthorhombic and was formed after heating to 885°C and cooling at 22°C.
The mean temperature of data collection was 23.2°C.

Additional patterns
PDF card 15-368

Reference
#1. Pistorius, C.W.F.T. and Pistorius, M.C. Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.(1962) 117,259.

d(A)	I^{rel}	hkl	2θ(°)
5.041	3	1 1 0	17.580
4.909	4	0 1 1	18.055
3.696	18	0 2 0	24.059
3.451	62	2 0 0	25.799
3.259	100	1 2 0	27.346
3.127	13	2 1 0	28.523
3.0049	94	0 1 2	29.707
2.9940	48	-1 1 2	29.818
2.8023	2	1 2 1	31.910
2.7092	21	-2 0 2	33.037
2.5658	11	1 1 2	34.941
2.5440	20	-2 1 2	35.250
2.5226	7	2 2 0	35.559
2.4992	2	-2 2 1	35.904
2.4509	2	-1 2 2	36.636
2.3451	7	-3 0 1	38.353
2.3215	4	1 3 0	38.758
2.3081	10	0 3 1	38.991
2.2432	20	-1 3 1	40.167
2.2352	16	-3 1 1	40.318
2.1971	1	3 1 0	41.047
2.1383	2	1 3 1	42.230
2.0629	38	2 1 2	43.852
2.0441	3	-3 1 2	44.275
2.0318	3	3 0 1	44.559
2.0053	2	2 3 0	45.179
1.9936	4	-2 3 1	45.459
1.9688	36	-1 3 2	46.065
1.9532	17	3 2 0	46.454
1.8855	3	0 2 3	48.225
1.8484	20	0 4 0	49.257
1.8435	15	-3 2 2	49.397
1.8311	24	1 3 2	49.753
1.8063	1	-3 0 3	50.485
1.7855	12	1 4 0	51.114
1.7497	1	-1 4 1	52.240
1.7255	4	4 0 0	53.027
1.6954	8	-4 0 2	54.044
1.6809	8	4 1 0	54.550
1.6667	2	3 1 2	55.055
1.6527	3	-4 1 2	55.562
1.6294	2	2 4 0	56.424
1.6103	8	-3 3 2	57.158
1.5977	5	-2 1 4+	57.651
1.5525	1	3 2 2	59.493
1.5412	2	-4 2 2	59.975
1.5367	5	-1 2 4+	60.169
1.5329	2	2 2 3	60.331
1.5272	1	-2 4 2	60.582
1.4552	1L	4 2 1	63.924
1.4516	1L	-3 4 1	64.098
1.4410	3	3 4 0	64.629
1.4323	1	3 0 3	65.069
1.4262	1L	-1 4 3	65.380
1.4083	8	1 2 4	66.318

continued

d(A)	I^{rel}	hkl	2θ(°)
1.4053	10	3 3 2	66.480
1.4018	5	4 0 2	66.666
1.3952	6	-3 4 2	67.024
1.3925	4	-5 1 1	67.173
1.3775	2	4 1 2	68.004

Strontium Titanium Phosphate, $SrTi_4(PO_4)_6$

Synonym
Strontium titanium orthophosphate

Sample
The sample was made by heating a 1:4:6 molar mixture of $SrCO_3$, TiO_2 (anatase), and $(NH_4)_2HPO_4$ at 500°C. It was then reground and heated to 1200°C overnight.

Color
Colorless

Symmetry classifications

Crystal System	Rhombohedral
Space Group	R**
Pearson Symbol	hR35

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	4.0° 2θ
$\sigma(I^{rel})$	±3

Crystallographic constants of this sample
(Hexagonal axes)
a = 8.2847 (3) A
c = 22.6000 (12)

c/a = 2.7279

V = 1343.36 A^3
Z = 3
Density (calc.) = 3.149 g/cm^3

Figures of merit
F_{30} = 212.0(.0040, 35)
M_{20} = 137.7

Comments
R** by analogy with other similar titanium phosphates. The structure is similar to $NaZr_2(PO_4)_3$. The temperature of data collection was approximately 25.0°C.

d(A)	I^{rel}	hkl	2θ(°)
7.531	7	0 0 3	11.742
6.840	20	1 0 1	12.932
6.058	2	0 1 2	14.611
4.439	11	1 0 4	19.988
4.144	39	1 1 0	21.424
3.824	8	0 1 5	23.240
3.766	2	0 0 6	23.605
3.630	100	1 1 3	24.505
3.543	5	0 2 1	25.116
3.419	6	2 0 2	26.039
3.0292	20	0 2 4	29.463
2.9446	3	1 0 7	30.330
2.8104	19	2 0 5	31.815
2.7871	79	1 1 6	32.089
2.6928	17	2 1 1	33.244
2.6374	8	1 2 2	33.963
2.6289	8	0 1 8	34.076
2.4441	2	2 1 4	36.742
2.3914	17	3 0 0	37.582
2.3249	6	1 2 5	38.698
2.2789	9	3 0 3	39.511
2.2192	4	2 0 8	40.621
2.1476	11	1 1 9	42.039
2.0766	10	2 1 7	43.547
2.0190	9	3 0 6	44.857
1.9971	4	2 2 3	45.376
1.9823	2	1 3 1	45.734
1.9753	2	0 1 11	45.904
1.9563	13	1 2 8	46.376
1.9119	2	0 2 10	47.520
1.8835	4	0 0 12	48.282
1.8773	4	1 3 4	48.450
1.8216	6	3 1 5	50.033
1.8146	24	2 2 6	50.237
1.7879	1	4 0 1	51.041
1.7825	1	2 0 11	51.207
1.7712	1	0 4 2	51.558
1.7359	6	2 1 10	52.688
1.7095	2	4 0 4	53.566
1.6937	4	1 3 7	54.103
1.6894	4	1 0 13	54.255
1.6668	1	0 4 5	55.051
1.6373	2	1 2 11	56.129
1.6267	9	3 1 8	56.528
1.5978	2	2 2 9	57.645
1.5803	3	3 2 4	58.345
1.5749	3	0 1 14	58.562
1.5654	13	4 1 0	58.955
1.5467	2	2 3 5	59.737
1.5329	2	4 1 3	60.332
1.5143	3	0 4 8	61.152
1.4935	5	1 3 10	62.099
1.4795	5	3 0 12	62.750
1.4721	9	2 0 14	63.102
1.4664	7	3 2 7	63.377
1.4458	9	4 1 6	64.386
1.4321	1	0 5 1	65.080
1.4295	1	3 1 11	65.211
1.4160	1	1 1 15	65.913
1.4053	1	4 0 10	66.479
1.3911	2	0 5 4	67.245
1.3873	4	1 2 14	67.458
1.3580	1L	3 3 3	69.115
1.3512	1	0 4 11	69.514
1.3092	1	1 3 13	72.081
1.2989	1	4 2 5	72.748
1.2964	2	3 3 6	72.908
1.2865	2	5 1 1	73.560

Tantalum Boride, TaB

CAS registry no.
12007-07-7

Sample
The sample which was obtained from STREM Chemicals, Inc. Newburyport, MA had approximately 7% Ta_3B_4 and TaB_2 present. Samples from several other sources were examined; they all had extra phases present.

Color
Very dark gray

Symmetry classifications

Crystal System	Orthorhombic
Space Group	Cmcm (63)
Pearson Symbol	oC8
Structure Type	CrB

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample
a = 3.28013 (12) A
b = 8.6708 (4)
c = 3.1557 (2)

a/b = 0.3783
c/b = 0.3639

V = 89.75 A^3
Z = 4
Density (calc.) = 14.191 g/cm^3

Figures of merit
F_{30} = 83.7(.0085, 42)
M_{20} = 162.5

Comments
The structure was studied by Kiessling (#1).
The mean temperature of data collection was 25.0°C.

Additional patterns
PDF 6-525

Reference
#1. Kiessling, R.
Acta Chem. Scand.(1949) 3,603.

d(A)	I^{rel}	hkl	2θ(°)
4.336	7	0 2 0	20.467
3.066	50	1 1 0	29.100
2.551	91	0 2 1	35.156
2.1989	100	1 1 1	41.013
2.1675	89	0 4 0	41.635
1.7865	30	0 4 1	51.085
1.6397	14	2 0 0	56.040
1.5777	17	0 0 2	58.449
1.5336	2	2 2 0+	60.304
1.4828	2	0 2 2	62.597
1.4451	5	0 6 0	64.421
1.4030	15	1 1 2	66.602
1.3791	68	1 5 1+	67.909
1.3137	9	0 6 1	71.796
1.3079	11	2 4 0	72.167
1.2758	32	1 3 2+	74.283
1.2082	6	2 4 1	79.220
1.1587	8	1 7 0	83.331
1.1371	8	2 0 2	85.283
1.0997	2	1 5 2+	88.930
1.0879	1	1 7 1	90.158
1.0846	5	3 1 0	90.501
1.0658	2	0 6 2	92.567
1.0254	14	2 6 1	97.395
1.0227	15	3 3 0	97.736
1.0070	6	2 4 2	99.807
0.9951	7	1 1 3	101.447
0.9728	1	3 3 1	104.722
0.9464	3	1 3 3	108.962
0.93390	8	1 7 2	111.141
0.92446	1	1 9 0	112.867
0.90417	1	2 8 0	116.847
0.89367	5	2 6 2	119.073
0.88709	9	1 9 1	120.534
0.86930	5	2 8 1	124.778
0.86741	14	1 5 3	125.258
0.85818	5	3 3 2	127.688
0.85045	2	0 6 3	129.851
0.82006	5	4 0 0	139.877
0.81969	2	2 4 3+	140.017

Tantalum Carbide, TaC

CAS registry no.
12070-06-3

Sample
The sample was obtained from Aesar Division of Johnson Matthey, Inc., Seabrook, NH.

Color
Dark brownish gray

Symmetry classifications

Crystal System	Cubic
Space Group	Fm3m (225)
Pearson Symbol	cF8
Structure Type	NaCl

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Ag
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±1

Crystallographic constants of this sample
a = 4.4547 (2) A

V = 88.40 A^3
Z = 4
Density (calc.) = 14.498 g/cm^3

Figures of merit
F_{10} = 97.4(.0103, 10)
M_{10} = 480.2

Comments
The structure was studied by van Arkel (#1).
The mean temperature of data collection was 24.0°C.

Additional patterns
PDF card 19-1292
Becker and Ebert (#2)
Schwartz and Summa (#3)

References

#1. van Arkel, A.E.
Physica (The Hague)(1924) 4,286.
#2. Becker, K. and Ebert, F.
Z. Phys.(1925) 31,268.
#3. Schwartz, M.V. and Summa, O.
Metallwirtsch., Metallwiss., Metalltech.(1933) 12,298.

d(A)	I^{rel}	hkl	2θ(°)
2.572	100	1 1 1	34.856
2.228	70	2 0 0	40.461
1.5750	41	2 2 0	58.561
1.3429	41	3 1 1	70.005
1.2858	14	2 2 2	73.611
1.1139	6	4 0 0	87.503
1.0219	10	3 3 1	97.845
0.9960	12	4 2 0	101.314
0.9094	3	4 2 2	115.782
0.85732	5	5 1 1	127.922

Titanium Boride, TiB_2

Synonym
Titanium diboride

CAS registry no.
12045-63-5

Sample
The sample was obtained from CERAC, Ino., Milwaukee, WI.

Color
Dark gray

Symmetry classifications

Crystal System	Hexagonal
Space Group	P6/mmm (191)
Pearson Symbol	hP3

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	4.0° 2θ
$\sigma(I^{rel})$	±4

Crystallographic constants of this sample

a = 3.03034 (8)
c = 3.22955 (8)

c/a = 1.0657

V = 25.68 A^3
Z = 1
Density (calc.) = 4.495 g/cm^3

Figures of merit

F_{21} = 172.2(.0057, 21)
M_{20} = 487.7

Comments
The structure was determined by Norton et al. (#1).
The temperature of data collection was approximately 25.0°C.

Additional patterns
PDF card 8-121

Reference
#1. Norton, J.T. et al.
Trans. Am. Inst. Min. Metall. Pet. Eng.(1949) 185,749.

d(A)	I^{rel}	hkl	2θ(°)
3.230	22	0 0 1	27.598
2.6247	55	1 0 0	34.133
2.0370	100	1 0 1	44.438
1.6145	12	0 0 2	56.992
1.5153	27	1 1 0	61.106
1.3751	16	1 0 2	68.134
1.3717	18	1 1 1	68.328
1.3122	7	2 0 0	71.895
1.2156	16	2 0 1	78.642
1.1049	14	1 1 2	88.400
1.0766	1L	0 0 3	91.367
1.01833	5	2 0 2	98.302
0.99589	8	1 0 3	101.334
0.99193	6	2 1 0	101.895
0.94821	13	2 1 1	108.656
0.87753	3	1 1 3	122.757
0.87472	5	3 0 0	123.436
0.84523	7	2 1 2	131.386
0.84437	3	3 0 1	131.644
0.83229	5	2 0 3	135.492
0.80739	1	0 0 4	145.131

Titanium Silicide, $TiSi_2$

Synonym
Titanium disilicide

CAS registry no.
12039-83-7

Sample
The sample was obtained from CERAC, Inc., Milwaukee, WI. The sample contained approximately 5% TiSi as a second phase.

Spectrographic analysis (wt.%, CERAC, Inc.)
0.1-0.6 Fe
0.1-0.3 Al
0.01-0.1 V
0.005-0.05 Ca, Co, Ni, Zr
0.001-0.01 Bi, B, Cr, Cu, K, Mn

Color
Very dark gray

Symmetry classifications

Crystal System	Orthorhombic
Space Group	Fddd (70)
Pearson Symbol	oF24

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Ag
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample
a = 8.2687 (5) A
b = 8.5534 (6)
c = 4.7983 (3)

a/b = 0.9667
c/b = 0.5610

V = 339.36 A^3
Z = 8
Density (calc.) = 4.074 g/cm^3

Figures of merit
F_{30} = 71.1(.0100, 42)
M_{20} = 126.6

Comments
The structure was determined by Laves and Walbaum (#1). It was later confirmed by Jeitschko (#2). Cotter et al. (#3) reported that $TiSi_2$ is dimorphous with the resultant structure depending on the method of synthesis.
The mean temperature of data collection was 23.5°C.

Additional patterns
PDF card 31-1405
PDF card 33-1384

Reference
#1. Laves, F. and Walbaum, H.J.
Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.(1939) 101,78.
#2. Jeitschko, W.
Acta Crystallogr., Sect. B(1977) 33, 2347.
#3. Cotter, P.G. et al.
J. Am. Ceram. Soc.(1956) 39,11.

d(A)	I^{rel}	hkl	2θ(°)
3.733	12	1 1 1	23.814
2.972	10	2 2 0	30.048
2.350	5	1 3 1	38.276
2.302	100	3 1 1	39.106
2.1382	43	0 4 0	42.231
2.0932	70	0 2 2	43.184
2.0666	2L	4 0 0	43.770
1.8319	45	3 3 1	49.730
1.5818	2	1 5 1	58.285
1.5441	2	1 1 3	59.849
1.5379	3	5 1 1	60.117
1.4890	3	2 4 2	62.308
1.4860	2	4 4 0	62.446
1.4703	2L	4 2 2	63.188
1.3912	15	3 5 1	67.241
1.3656	14	3 1 3	68.675
1.3475	2L	2 6 0	69.730
1.3116	11	6 2 0	71.930
1.2447	9	3 3 3	76.465
1.2257	12	0 6 2	77.870
1.1998	7	0 0 4	79.889
1.1951	10	6 0 2	80.262
1.1720	2L	1 7 1	82.180
1.1125	2L	2 2 4	87.640
1.0879	5	3 7 1	90.150
1.0756	5	3 5 3	91.477
1.0693	4	0 8 0	92.167
1.0661	2	5 3 3	92.534
1.0541	2	4 6 2	93.905
1.0461	6	0 4 4	94.840
1.0431	7	6 4 2	95.207
1.0377	2	4 0 4	95.861
1.0336	2	8 0 0	96.356
0.9909	2	6 6 0	102.046
0.9268	2L	8 2 2	112.432
0.9158	2	3 7 3+	114.512
0.90150	2	7 3 3	117.401
0.89734	3	9 1 1	118.281
0.88521	3	6 2 4	120.962
0.88301	3	4 8 2+	121.468

Tungsten Boride, δ-WB

CAS registry no.
12007-09-9

Sample
The sample was obtained from the Materials Research Corp., West Nyack, NY.

Color
Dark gray

Symmetry classifications
Crystal System Tetragonal
Space Group $I4_1/amd$ (141)
Pearson Symbol tI16

Data collection and analysis parameters
Radiation $CuK\alpha_1$
Wavelength 1.5405981 A
2θ Standard W
Scanned to 4.0° 2θ
$\sigma(I^{rel})$ ±4

Crystallographic constants of this sample
a = 3.11655 (11) A
c = 16.9101 (8)

c/a = 5.4259

V = 164.25 A^3
Z = 8
Density (calc.) = 15.744 g/cm^3

Figures of merit
F_{30} = 77.4(.011, 35)
M_{20} = 168.7

Comments
The structure was determined by Kiessling (#1).
There is an orthorhombic high temperature form (#2).
The temperature of data collection was approximately 25.0°C.

Additional patterns
PDF card 6-0635

References
#1. Kiessling, R.
Acta Chem. Scand.(1947) 1,893.
#2. Post, B. and Glasser, F.W.
J. Chem. Phys.(1952) 20,1050.

d(A)	I^{rel}	hkl	2θ(°)
4.227	11	0 0 4	21.002
3.063	20	1 0 1	29.127
2.727	90	1 0 3	32.813
2.292	87	1 0 5	39.282
2.133	100	1 1 2	42.338
2.114	34	0 0 8	42.741
1.9095	29	1 0 7	47.583
1.7362	18	1 1 6	52.676
1.6095	1	1 0 9	57.189
1.5581	26	2 0 0	59.260
1.4625	2	2 0 4	63.567
1.4094	5	0 0 12	66.262
1.3892	4	2 1 1	67.349
1.3788	5	1 0 11	67.930
1.3530	19	2 1 3	69.405
1.3416	35	1 1 10	70.080
1.2884	23	2 1 5	73.433
1.2541	20	2 0 8	75.788
1.2073	12	2 1 7	79.291
1.2005	10	1 0 13	79.830
1.1016	7	2 2 0	88.731
1.0659	1	2 2 4	92.548
1.0600	7	1 0 15	93.218
1.0569	5	0 0 16	93.577
1.0451	7	2 0 12	94.958
1.0366	1L	3 0 1	95.999
1.0324	3	2 1 11	96.510
1.0217	3	3 0 3	97.871
0.9929	5	3 0 5	101.755
0.9790	12	3 1 2	103.778
0.9773	17	2 2 8	104.038
0.9543	2	3 0 7	107.637
0.9511	2	2 1 13	108.178
0.9475	10	1 0 17	108.774
0.9303	5	3 1 6	111.788
0.87637	13	2 1 15	123.036
0.87464	11	2 0 16	123.455
0.86805	5	2 2 12	125.094
0.86421	13	1 1 18	126.082
0.85435	6	3 2 3	128.743
0.85151	21	3 1 10	129.547

Tungsten Carbide, α-W_2C

CAS registry no.
12070-13-2

Sample
The sample was obtained from CERAC, Inc., Milwaukee, WI.

Color
Dark gray

Symmetry classifications

Crystal System	Hexagonal
Space Group	$P\bar{3}m1$ (164)
Pearson Symbol	hP3

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	W
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±1

Crystallographic constants of this sample
a = 2.99704 (9) A
c = 4.7279 (3)

c/a = 1.5775

V = 36.78 A^3
Z = 1
Density (calc.) = 17.144 g/cm^3

Figures of merit
F_{22} = 93.0(.0085, 28)
M_{20} = 250.2

Comments
The structure was determined by Metcalfe (#1).
β-W_2C, with an orthorhombic superlattice cell 4 times the volume of the hexagonal cell above, was made by Rudy and Windisch (#2) by quenching W_2C from above 2000°C.
The mean temperature of data collection was 23.5°C.

Additional patterns
PDF card 2-1134
PDF card 20-1315

References
#1. Metcalfe, A.G.
J. Inst. Met.(1947) 73,591.
#2. Rudy, E. and Windisch, S.
J. Am. Ceram. Soc.(1967) 50,272.

d(A)	I^{rel}	hkl	2θ(°)
2.596	25	1 0 0	34.524
2.364	22	0 0 2	38.029
2.2757	100	1 0 1	39.569
1.7478	17	1 0 2	52.300
1.4986	14	1 1 0	61.861
1.3469	14	1 0 3	69.769
1.2975	2	2 0 0	72.839
1.2657	12	1 1 2	74.979
1.2514	10	2 0 1	75.984
1.1821	2	0 0 4	81.328
1.1377	3	2 0 2	85.228
1.0756	2	1 0 4	91.472
1.0018	3	2 0 3	100.510
0.9811	1L	2 1 0	103.472
0.9607	5	2 1 1	106.614
0.92812	3	1 1 4	112.189
0.90609	1	2 1 2	116.452
0.88840	2	1 0 5	120.239
0.87384	1	2 0 4	123.650
0.86514	1	3 0 0	125.841
0.83287	3	2 1 3	135.299
0.81244	2	3 0 2	142.932

Vanadium Carbide, V_8C_7

CAS registry no.
1207-10-9

Sample
The sample was obtained from Aesar Division of Johnson Matthey, Inc., Seabrook, NH.

Color
Very dark gray

Symmetry classifications

Crystal System	Cubic
Space Group	$P4_132$ (213)
Pearson Symbol	cP60

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standards	FP Si
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±1

Crystallographic constants of this sample
a = 8.33409 (11) Å

V = 578.86 A^3
Z = 4
Density (calc.) = 5.641 g/cm^3

Figures of merit
F_{30} = 64.9(.0091, 51)
M_{20} = 96.0

Comments
The symmetry classification was given by de Novion et al. (#1). The stronger reflections can be indexed on a subcell, NaCl type, having a=4.167 A.
The mean temperature of data collection was 22.2°C.

Additional patterns
PDF card 23-1468
PDF card 25-1002
Kordes (#2)

References

#1. de Novion, C. et al.
C. R. Seances Acad. Sci., Ser. B(1966) 263B,775.
#2. Kordes, D.
Phys. Status Solidi (1969) 26,K103

d(A)	I^{rel}	hkl	2θ(°)
5.893	3	1 1 0	15.022
4.814	2	1 1 1	18.414
3.728	4	2 1 0	23.848
3.404	2	2 1 1	26.157
2.514	1L	3 1 1	35.690
2.405	94	2 2 2	37.358
2.311	3	3 2 0	38.943
2.2282	1L	3 2 1	40.450
2.0829	100	4 0 0	43.410
1.9642	1	3 3 0	46.178
1.8180	1	4 2 1	50.137
1.7766	1L	3 3 2	51.389
1.6346	1	5 1 0	56.230
1.6037	1	5 1 1	57.414
1.5475	4	5 2 0	59.707
1.5212	2	5 2 1	60.846
1.4733	56	4 4 0	63.045
1.2860	1	5 4 1	73.595
1.2563	34	6 2 2	75.634
1.2425	4	6 3 0	76.627
1.2287	1L	6 3 1	77.645
1.2028	17	4 4 4	79.649
1.1785	1L	5 5 0	81.634
1.1670	1	5 5 1	82.612
1.1446	2	7 2 0	84.593
1.1340	1	7 2 1	85.576
1.0944	1L	7 3 0	89.469
1.0851	1L	7 3 1	90.450
1.0670	1	6 5 0	92.424
1.0585	1L	6 5 1	93.395
1.0419	9	8 0 0	95.351
1.0258	1L	7 4 1	97.337
1.0183	1L	7 3 3	98.303
1.0034	2	7 4 2	100.299
0.9688	1	7 5 0	105.324
0.9624	1	7 5 1	106.341
0.9560	15	6 6 2	107.369
0.9498	1	8 3 2	108.389
0.9317	25	8 4 0	111.530
0.92032	1L	9 1 0	113.648
0.90396	3	7 6 0	116.890
0.89870	2	7 6 1	117.990
0.87841	1	7 5 4	122.547
0.86413	2	8 5 2	126.103
0.85962	2	9 3 2	127.298
0.85059	22	8 4 4	129.810
0.84188	1	7 7 0	132.406
0.83763	1L	7 7 1	133.741
0.82926	5	10 1 0	136.526
0.82517	1L	10 1 1	137.975
0.80951	1L	9 5 0	144.188
0.80569	1	9 5 1	145.910
0.80196	14	10 2 2	147.693

Vanadium Nitride, VN

CAS registry no.
24646-85-3

Sample
The sample was obtained from CERAC, Inc., Milwaukee, WI.

Spectrographic analysis (wt.%, CERAC, Inc.)
0.01-0.1 Al, Si, Zr
0.005-0.05 Fe, Mg
0.001-0.01 Bi, Ca, Cr, Cu, Mn, Nb, Ni, Sn, Ti

Color
Brownish black

Symmetry classifications

Crystal System	Cubic
Space Group	Fm3m (225)
Pearson Symbol	cF8
Structure Type	NaCl

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	W
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample
a = 4.13916 (4) A

V = 70.91 A^3
Z = 4
Density (calc.) = 6.083 g/cm^3

Figures of merit
F_9 = 454.0(.0022, 9)
M_9 is greater than 1000.

Comments
The structure was studied by Becker and Ebert (#1).
The mean temperature of data collection was 23.3°C.

Additional patterns
PDF card 25-1252

Reference
#1. Becker, K. and Ebert, F.
Z. Phys.(1925) 31,268.

d(A)	I^{rel}	hkl	2θ(°)
2.3896	66	1 1 1	37.611
2.0698	100	2 0 0	43.697
1.46338	40	2 2 0	63.523
1.24804	17	3 1 1	76.225
1.19486	11	2 2 2	80.283
1.03478	3	4 0 0	96.217
0.94959	2	3 3 1	108.425
0.92553	8	4 2 0	112.667
0.84491	7	4 2 2	131.481

Yttrium Nitride, YN

CAS registry no.
25764-13-0

Sample
The sample was obtained from Alfa Products, Thiokol/Ventron Division, Danvers, MA. It was run in a dry atmosphere because of its sensitivity to humidity.

Color
Black

Symmetry classifications

Crystal System	Cubic
Space Group	Fm3m (225)
Pearson Symbol	cF8

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±1

Crystallographic constants of this sample
a = 4.8944 (2) A

V = 117.25 A^3
Z = 4
Density (calc.) = 5.830 g/cm^3

Figures of merit
F_{12} = 80.9(.0124, 12)
M_{12} = 386.6

Comments
The structure was determined by Kempter et al. (#1).
The mean temperature of data collection was 23.5°C.

Additional patterns
Kempter et al. (#1)

Reference
#1. Kempter, C.P., Kirikorian, N.H., and McGuire, J.C. J. Phys. Chem.(1957) 61,1237.

d(A)	I^{rel}	hkl	2θ(°)
2.825	100	1 1 1	31.645
2.447	86	2 0 0	36.704
1.7298	46	2 2 0	52.887
1.4754	28	3 1 1	62.948
1.4126	13	2 2 2	66.093
1.2237	5	4 0 0	78.023
1.1226	8	3 3 1	86.654
1.0946	10	4 2 0	89.456
0.9990	8	4 2 2	100.896
0.9419	5	5 1 1	109.725
0.86528	2	4 4 0	125.804
0.82730	6	5 3 1	137.214

Zinc Molybdenum Oxide, α-$ZnMoO_4$

Synonym
Zinc molybdate
Molybdenum zinc tetraoxide

CAS registry no.
13767-32-3

Sample
The sample was prepared by heating an equimolar mixture of ZnO and MoO_3 at 650°C for 20 hours with periodic grinding.

Color
Colorless

Symmetry classifications
Crystal System Triclinic
Space Group $P\bar{1}$ (2)
Pearson Symbol aP36

Data collection and analysis parameters
Radiation $CuK\alpha_1$
Wavelength 1.5405981 A
2θ Standard Ag
Scanned to 5.0° 2θ
$\sigma(I^{rel})$ ±3

Crystallographic constants of this sample
a = 8.3678 (8) A
b = 9.6916 (8)
c = 6.9643 (6)
α = 106.872 (8)°
β = 101.726 (8)
γ = 96.734 (8)

a/b = 0.8634
c/b = 0.7186

V = 519.75 A^3
Z = 6
Density (calc.) = 4.319 g/cm^3

Figures of merit
F_{30} = 104.7(.0073, 39)
M_{20} = 45.3

Comments
The structure was determined by Abrahams (#1).
A monoclinic polymorph of $ZnMoO_4$ is reported by Young and Schwartz (#2).
The mean temperature of data collection was 23.9°C.

Additional patterns
PDF card 25-1023

References
#1. Abrahams, S.C.
J. Chem. Phys.(1967) 46,2052.
#2. Young, A.P. and Schwartz, C.M.
Science (Washington, D.C.)(1963) 141,348.

d(A)	I^{rel}	hkl	2θ(°)
9.11	6	0 1 0	9.702
6.692	6	-1 1 0	13.219
6.455	5	0 0 1	13.707
5.537	13	1 1 0	15.994
5.270	4	-1 -1 1	16.810
4.720	4	1 -1 1	18.784
4.611	15	0 1 1	19.235
4.580	14	-1 1 1	19.367
4.555	17	0 2 0	19.472
4.512	6	1 0 1	19.659
4.329	5	-1 2 0	20.498
4.024	7	2 0 0	22.070
3.969	12	-2 1 0	22.384
3.923	16	1 -2 1	22.650
3.879	34	-2 0 1+	22.911
3.678	89	1 2 0	24.177
3.599	12	1 1 1	24.717
3.551	4	-2 1 1	25.055
3.450	14	2 1 0	25.806
3.408	61	0 -1 2	26.130
3.381	45	-1 -1 2	26.336
3.344	100	-2 2 0	26.634
3.293	18	-1 0 2	27.055
3.260	14	0 2 1	27.333
3.230	29	2 -1 1+	27.598
3.171	19	0 -3 1	28.122
3.157	18	0 -2 2	28.241
3.088	8	2 0 1	28.894
3.061	15	-1 -2 2	29.152
3.037	6	0 3 0+	29.384
3.005	7	2 -2 1	29.701
2.971	31	-2 -2 1	30.055
2.941	4	1 -1 2	30.367
2.894	4	-2 0 2	30.871
2.873	5	-1 1 2	31.101
2.832	6	1 -2 2	31.562
2.778	18	1 2 1	32.194
2.773	19	0 1 2	32.254
2.766	20	1 0 2+	32.340
2.716	8	-3 1 0	32.957
2.681	35	3 0 0	33.389
2.644	29	-2 1 2	33.877
2.634	14	-2 -2 2	34.008
2.585	5	2 -3 1	34.677
2.581	6	-1 -3 2	34.734
2.533	6	-1 3 1	35.413
2.5165	14	1 -3 2	35.649
2.4579	9	0 3 1	36.528
2.4506	9	3 1 0	36.641
2.4259	4	1 1 2	37.028
2.4050	16	0 -4 1+	37.361
2.3960	13	-1 2 2	37.506
2.3832	5	2 -1 2	37.715
2.3571	6	2 -2 2	38.150
2.3384	7	-3 -1 2	38.467

continued

d(Å)	I^{rel}	hkl	2θ(°)
2.3084	15	-1 4 0	38.986
2.2867	7	-3 -2 1+	39.371
2.2832	10	3 0 1	39.434
2.2766	6	0 4 0+	39.554
2.2631	4	-1 -2 3+	39.800
2.2566	4	2 0 2	39.919
2.2295	14	-3 3 0+	40.425
2.2208	11	-1 0 3	40.590
2.2035	2	1 3 1	40.923
2.1924	3	2 -3 2	41.139
2.1671	10	2 -4 1	41.643
2.1638	10	-2 4 0	41.709
2.1561	3	1 -4 2	41.865
2.1505	3	0 0 3	41.979
2.1416	4	3 2 0+	42.161
2.1316	4	-2 0 3	42.370
2.1260	4	3 -3 1	42.485
2.1054	2	0 -3 3	42.923
2.0958	7	-1 -3 3	43.128
2.0902	10	1 4 0	43.249
2.0872	8	-3 3 1	43.315
2.0744	11	1 -2 3+	43.595
2.0708	9	1 2 2	43.675
2.0477	3	-4 1 0+	44.195
2.0300	19	-1 1 3	44.601
2.0161	2	-1 4 1	44.925
1.9950	2	-1 3 2	45.427
1.9831	7	-4 -1 1+	45.713
1.9748	1	-2 -4 1	45.918
1.9594	21	1 0 3+	46.299
1.9546	20	-4 2 1	46.419
1.9494	8	-3 -1 3+	46.550
1.9409	11	-2 -4 2	46.767
1.9377	11	-4 0 2+	46.847
1.9296	6	-3 0 3	47.057
1.9235	6	-3 4 0+	47.214
1.8989	10	2 3 1+	47.863
1.8927	10	3 -4 1	48.031
1.8841	6	-3 -2 3	48.264
1.8650	1	0 -5 2	48.791
1.8479	7	3 2 1+	49.271
1.8418	7	4 -2 1	49.445
1.8390	5	2 4 0	49.527
1.8315	1	-3 1 3	49.744
1.8259	3	-4 -2 1+	49.905
1.8218	2	0 5 0	50.027
1.8063	6	1 4 1	50.484
1.7983	6	-3 4 1+	50.727
1.7912	10	-2 5 0+	50.941

Zinc Nitride, Zn_3N_2

CAS registry no.
1313-49-1

Sample
The sample was obtained from Alfa Products, Thiokol/Ventron Division, Danvers, MA. It contained a small amount of ZnO.

Color
Black

Symmetry classifications

Crystal System	Cubic
Space Group	Ia3 (206)
Pearson Symbol	cI80

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Ag
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±1

Crystallographic constants of this sample
a = 9.77687 (14) A

V = 934.54 A^3
Z = 16
Density (calc.) = 6.373 g/cm^3

Figures of merit
F_{30} = 84.5(.0108, 33)
M_{20} = 128.1

Comments
The structure was determined qualitatively by Juza and Hahn (#1).
The mean temperature of data collection was 24.3°C.

Additional patterns
PDF card 10-256

Reference
#1. Juza, R. and Hahn, H.
Z. Anorg. Allg. Chem.(1940) 244,125.

d(A)	I^{rel}	hkl	2θ(°)
3.991	11	2 1 1	22.255
3.456	1	2 2 0	25.754
2.824	12	2 2 2	31.657
2.614	100	3 2 1	34.280
2.445	89	4 0 0	36.728
2.305	1	4 1 1	39.046
2.186	1L	4 2 0	41.270
2.0847	63	3 3 2	43.370
1.9957	1L	4 2 2	45.410
1.9176	3	4 3 1	47.368
1.7853	7	5 2 1	51.122
1.7286	67	4 4 0	52.925
1.6297	2	6 0 0	56.414
1.5861	4	6 1 1	58.112
1.5458	1L	6 2 0	59.777
1.5088	1	5 4 1	61.400
1.4741	2	6 2 2	63.010
1.4411	4	6 3 1	64.623
1.4113	9	4 4 4	66.159
1.3830	3	5 4 3	67.695
1.3552	1	6 4 0	69.278
1.3307	26	7 2 1	70.745
1.3066	1L	6 4 2	72.252
1.2418	18	6 5 1	76.680
1.2221	4	8 0 0	78.145
1.2032	1L	7 4 1	79.616
1.1859	1L	6 4 4	81.017
1.1522	1L	6 6 0	83.908
1.1370	1L	7 4 3	85.299
1.1216	1L	6 6 2	86.750
1.1071	5	7 5 2	88.179
1.0932	4	8 4 0	89.601
1.0543	6	9 2 1	93.881
1.0422	1	6 6 4	95.309
1.0306	1	8 5 1	96.737
1.0085	3	9 3 2	99.609
0.9979	4	8 4 4	101.060
0.9875	1	9 4 1	102.536
0.9812	1L	0 0 0	103.456
0.9680	3	10 1 1	105.456
0.9496	1L	9 4 3	108.424
0.9321	5	10 3 1	111.455
0.9077	1L	10 4 0	116.122
0.9000	1	9 6 1	117.713
0.87094	4	10 5 1	124.367
0.86416	1L	8 8 0	126.096
0.84455	4	9 7 2	131.590
0.83832	1L	10 6 0	133.519
0.83225	1L	11 4 1	135.505
0.82050	1	9 6 5	139.707
0.80919	1	9 8 1	144.329
0.79825	3	10 7 1	149.584
0.79300	1	12 2 2	152.512

Zirconium Carbide, ZrC

CAS registry no.
12070-14-3

Sample
The sample was obtained from Aesar Division of Johnson Matthey, Inc., Seabrook, NH.

Color
Very dark gray

Symmetry classifications

Crystal System	Cubic
Space Group	Fm3m (225)
Pearson Symbol	cF8
Structure Type	Isostructural with NaCl

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	W
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±2

Crystallographic constants of this sample
a = 4.6930 (2) A

V = 103.36 A^3
Z = 4
Density (calc.) = 6.634 g/cm^3

Figures of merit
F_{11} = 115.2(.0087, 11)
M_{11} = 577.6

Comments
The structure was studied by van Arkel (#1).
The mean temperature of data collection was 24.0°C.

Additional patterns
PDF card 19-1487
Sedivy et al. (#2)

References
#1. van Arkel, A.E.
Physica (The Hague)(1924) 4,286.
#2. Sedivy et al.
Freiberg. Forschungsh. B(1968) B,95.

d(A)	I^{rel}	hkl	2θ(°)
2.709	100	1 1 1	33.041
2.346	82	2 0 0	38.338
1.6592	62	2 2 0	55.325
1.4149	50	3 1 1	65.969
1.3547	19	2 2 2	69.306
1.1735	10	4 0 0	82.051
1.0768	20	3 3 1	91.340
1.0494	23	4 2 0	94.455
0.9579	17	4 2 2	107.061
0.90312	15	5 1 1	117.064
0.82961	6	4 4 0	136.405

Zirconium Nitride, ZrN

CAS registry no.
25658-42-8

Sample
The sample was obtained from A. D. Mackay, Inc., New York City. It also contained a small amount of zirconium.

Symmetry classifications

Crystal System	Cubic
Space Group	Fm3m (225)
Pearson Symbol	cF8

Data collection and analysis parameters

Radiation	$CuK\alpha_1$
Wavelength	1.5405981 A
2θ Standard	Si
Scanned to	5.0° 2θ
$\sigma(I^{rel})$	±1

Crystallographic constants of this sample
a = 4.57756 (10) A

V = 95.92 A^3
Z = 4
Density (calc.) = 7.287 g/cm^3

Figures of merit
F_{11} = 203.7(.0049, 11)
M_{11} is greater than 1000.

Comments
The structure was qualitatively determined by Houska (#1).
The mean temperature of data collection was 23.7°C.

Additional patterns
PDF card 2-956
PDF card 31-1493
Swanson et al. (#2)

Reference
#1. Houska, C. R.
J. Phys. Chem. Solids, 25, 359.
#2. Swanson, H. E., McMurdie, H. F., Morris, M. C. and Evans, E. H.
Natl. Bur. Stand. (U. S.) Monogr. 25, 5, 80.

d(A)	I^{rel}	hkl	2θ(°)
2.6430	100	1 1 1	33.890
2.2891	74	2 0 0	39.329
1.6186	36	2 2 0	56.835
1.3802	24	3 1 1	67.852
1.3214	9	2 2 2	71.314
1.1444	2	4 0 0	84.611
1.05016	5	3 3 1	94.362
1.02369	6	4 2 0	97.610
0.93441	3	4 2 2	111.049
0.88096	3	5 1 1	121.944
0.80918	3	4 4 0	144.333

The multi-volume cumulative indices will be published in 1986 and every other year thereafter.

The mineral name index for this issue follows.

Mineral Name Index, Sec. 21

*Natural mineral.

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NBS-114A (REV. 2-8C)

U.S. DEPT. OF COMM. **BIBLIOGRAPHIC DATA SHEET** (See instructions)	1. PUBLICATION OR REPORT NO. NBS/MN-25/Sec.21	2. Performing Organ. Report No.	3. Publication Date September 1985

4. TITLE AND SUBTITLE

Standard X-ray Diffraction Powder Patterns
Section 21 - Data for 92 Substances

5. AUTHOR(S) M. C. Morris, H. F. McMurdie, E. H. Evans, B. Paretzkin, H. S. Parker, C. R. Hubbard, W. Wong-Ng, and D. Gladhill

6. PERFORMING ORGANIZATION (If joint or other than NBS, see instructions)

NATIONAL BUREAU OF STANDARDS
U.S. DEPARTMENT OF COMMERCE
GAITHERSBURG, MD 20899

7. Contract/Grant No.

8. Type of Report & Period Covered
Final

9. SPONSORING ORGANIZATION NAME AND COMPLETE ADDRESS (Street, City, State, ZIP)

JCPDS - International Centre
for Diffraction Data
1601 Park Lane
Swarthmore, PA 19081

10. SUPPLEMENTARY NOTES

Library of Congress Catalog Card Number: 53-61386

☐ Document describes a computer program; SF-185, FIPS Software Summary, is attached.

11. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)

Standard x-ray powder diffraction patterns are presented for 92 substances. These patterns, useful for identification, were obtained by automated diffractometer methods. The lattice constants from the experimental work were refined by least-squares methods, and reflections were assigned hkℓ indices consistent with space group extinctions. Relative intensities, calculated densities, literature references, and other relevant data are included.

12. KEY WORDS (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)

crystal structure; densities; lattice constants; powder patterns; relative intensities; standard; x-ray diffraction.

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14. NO. OF PRINTED PAGES
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